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* * * * * * * * * * Welcome to STN International * * * * * * * * * * * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 JAN 08 CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3 JAN 16 CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 4 JAN 16 IPC version 2007.01 thesaurus available on STN
NEWS 5 JAN 16 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6 JAN 22 CA/CAplus updated with revised CAS roles
NEWS 7 JAN 22 CA/CAplus enhanced with patent applications from India
NEWS 8 JAN 29 PHAR reloaded with new search and display fields
NEWS 9 JAN 29 CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10 FEB 15 PATDPASPC enhanced with Drug Approval numbers
NEWS 11 FEB 15 RUSSIAPAT enhanced with pre-1994 records
NEWS 12 FEB 23 KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13 FEB 26 MEDLINE reloaded with enhancements
NEWS 14 FEB 26 EMBASE enhanced with Clinical Trial Number field
NEWS 15 FEB 26 TOXCENTER enhanced with reloaded MEDLINE
NEWS 16 FEB 26 IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17 FEB 26 CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 18 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19 MAR 16 CASREACT coverage extended
NEWS 20 MAR 20 MARPAT now updated daily
NEWS 21 MAR 22 LWPI reloaded
NEWS 22 MAR 30 RDISCLOSURE reloaded with enhancements
NEWS 23 APR 02 JICST-EPLUS removed from database clusters and STN
NEWS 24 APR 30 GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25 APR 30 CHEMCATS enhanced with 1.2 million new records
NEWS 26 APR 30 CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 27 APR 30 INPADOC replaced by INPADOCDB on STN
NEWS 28 MAY 01 New CAS web site launched

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

| | |
|------------|---|
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
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FILE 'REGISTRY' ENTERED AT 11:51:54 ON 07 MAY 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6
DICTIONARY FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6

New CAS Information Use Policies. enter HELP USAGETERMS for details.

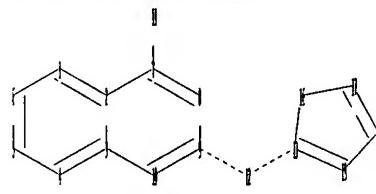
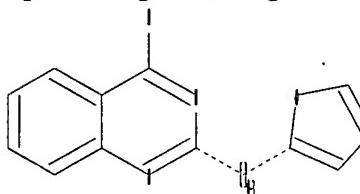
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stn/gen/stndoc/properties.html>

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Uploading C:\Program Files\Stnexp\Queries\10567660.str



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chain nodes :  
11 12  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 13 16 17 18 19  
chain bonds :  
7-11 9-12 12-13  
ring bonds :  
1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10 13-16 13-19 16-17 17-18  
18-19  
exact/norm bonds :  
7-11 9-12 12-13  
exact bonds :  
13-16 13-19 16-17 17-18 18-19  
normalized bonds :  
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isolated ring systems :  
containing 1 : 13 :
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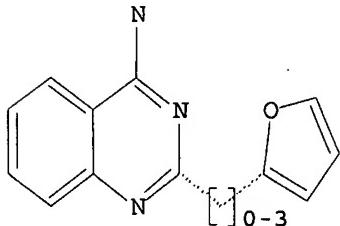
10/ 567,660

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 13:Atom 16:Atom 17:Atom 18:Atom 19:Atom

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 sample
SAMPLE SEARCH INITIATED 11:52:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5 TO 234
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s 11 ful
FULL SEARCH INITIATED 11:52:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 157 TO ITERATE

100.0% PROCESSED 157 ITERATIONS 104 ANSWERS
SEARCH TIME: 00.00.01

L3 104 SEA SSS FUL L1

=> file zcaplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
172.10 172.31

FILE 'ZCAPPLUS' ENTERED AT 11:52:30 ON 07 MAY 2007
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FILE COVERS 1907 - 7 May 2007 VOL 146 ISS 20
FILE LAST UPDATED: 6 May 2007 (20070506/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 40 L3

=> d his

(FILE 'HOME' ENTERED AT 11:51:17 ON 07 MAY 2007)

FILE 'REGISTRY' ENTERED AT 11:51:54 ON 07 MAY 2007
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L3 104 S L1 FUL

FILE 'ZCPLUS' ENTERED AT 11:52:30 ON 07 MAY 2007
L4 40 S L3

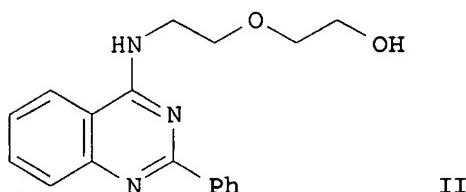
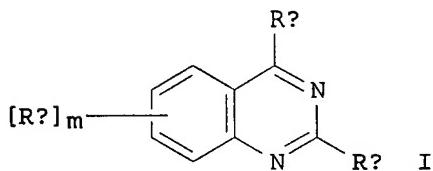
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YOU HAVE REQUESTED DATA FROM 40 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:655778 ZCPLUS
DOCUMENT NUMBER: 145:124592
TITLE: Preparation of quinazoline derivatives for the treatment and prevention of diabetes and obesity
INVENTOR(S): Lee, Nam Kyu; Lee, Jun Won; Lee, Sukho; Im, Guang-Jin; Han, Hye Young; Kim, Tae Kon; Kim, Yong Hyuk; Kwak, Wie-Jong; Kim, Sang Woong; Ha, Joohun; Kim, Eon Kyum; Lee, Jung Kyu; Yoo, Choong Yeul; Lee, Dae Yeon
PATENT ASSIGNEE(S): SK Chemicals, Co., Ltd., S. Korea; Leadgenex Inc.; Industry Academic Cooperation Foundation of Kyunghee University
SOURCE: PCT Int. Appl., 163 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| WO 2006071095 | A1 | 20060706 | WO 2005-KR4664 | 20051230 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, | | | | |

YU, ZA, ZM, ZW
 RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM

KR 2006079121 A 20060705 KR 2005-134722 20051230
 PRIORITY APPLN. INFO.: KR 2004-117708 A 20041231
 OTHER SOURCE(S): MARPAT 145:124592
 GI



AB The invention is related to the preparation of quinazolines I [Ra, Rb= independently H, (un)substituted alk(en/yn)yl, hetero/aryl, etc.; m = 0-4; each Rc = independently H, halo, CF₃, CN, OH, SH, NH₂, (un)substituted hetero/aryl, alkylthio, alkanoyloxy, etc.; any identical or different substituents of hetero/aryl or heterocyclyl of Rc may bond with each other to form -CH:CH-CH:CH-, -N:CH-CH:CH-, -CH:CH-O-, -S-CH:CH-, etc.] (e.g., II), and their pharmaceutically acceptable salts, that are effective in lowering blood glucose level and body weight, and to their use as active ingredients in pharmaceutical compns. useful for treatment and/or prevention of diabetes and/or obesity. Four general prepns. are given. An increase of AMPK activity was observed when the C2C12 muscle cells were treated with quinazolines I. A significant decrease in blood glucose level and body weight was observed in db/db mice after 10 days of oral or abdominal administration, demonstrating their preventive and therapeutic effect for diabetes and obesity.

IT 496872-97-0P, [2-(Furan-2-yl)quinazolin-4-yl] (3,4,5-trimethoxybenzyl)amine 553656-88-5P, [2-(Furan-2-yl)quinazolin-4-yl] (4-methoxybenzyl)amine 896726-60-6P, [2-(Furan-2-yl)quinazolin-4-yl] (2-methoxybenzyl)amine 896726-61-7P, [2-(Furan-2-yl)quinazolin-4-yl] (3-methoxybenzyl)amine 896726-62-8P, [(Benzodioxol-5-yl)methyl] [2-(furan-2-yl)quinazolin-4-yl]amine 896726-63-9P, (2,3-Dimethoxybenzyl) [2-(furan-2-yl)quinazolin-4-yl]amine 896726-64-0P, (3,5-Dimethoxybenzyl) [2-(furan-2-yl)quinazolin-4-yl]amine 896726-65-1P, (3,4-Dimethoxybenzyl) [2-(furan-2-yl)quinazolin-4-yl]amine 896726-66-2P, (2,4-Dimethoxybenzyl) [2-(furan-2-yl)quinazolin-4-yl]amine 896726-67-3P, (2,5-Dimethoxybenzyl) [2-(furan-2-yl)quinazolin-4-yl]amine 896726-68-4P, [2-(Furan-2-yl)quinazolin-4-yl] (2,4,6-trimethoxybenzyl)amine

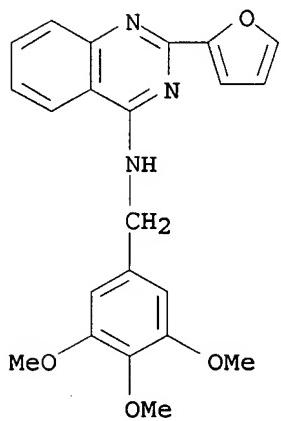
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(glucose lowering agent; preparation of quinazolines for treatment and prevention of diabetes and obesity)

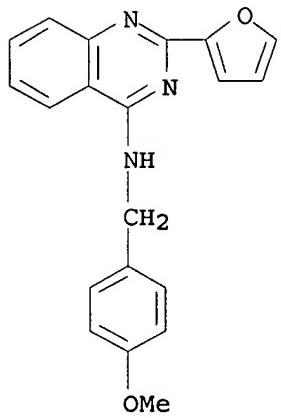
RN 496872-97-0 ZCPLUS

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(CA INDEX NAME)



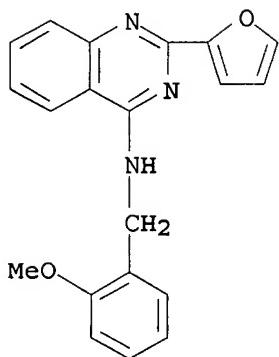
RN 553656-88-5 ZCPLUS

CN 4-Quinazolinamine, 2-(2-furanyl)-N-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



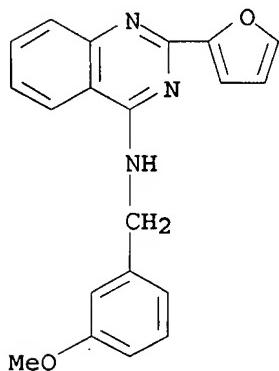
RN 896726-60-6 ZCPLUS

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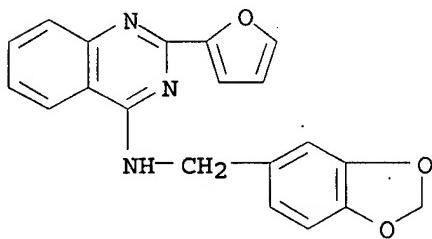
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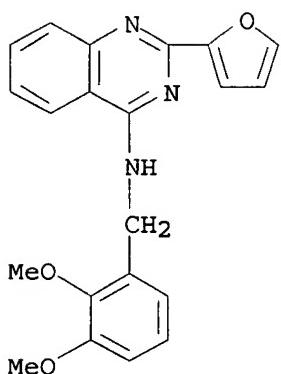
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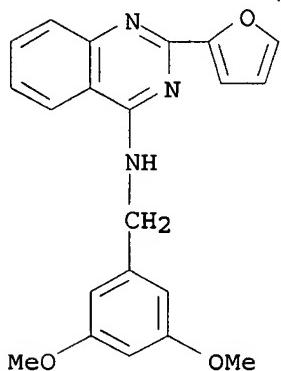
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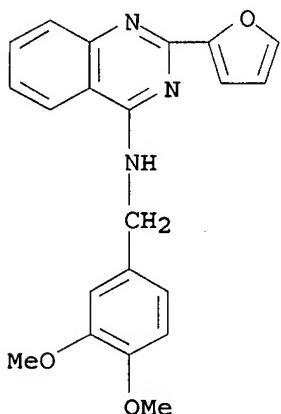
RN 896726-64-0 ZCPLUS

CN 4-Quinazolinamine, N-[(3,5-dimethoxyphenyl)methyl]-2-(2-furanyl)- (9CI)
(CA INDEX NAME)



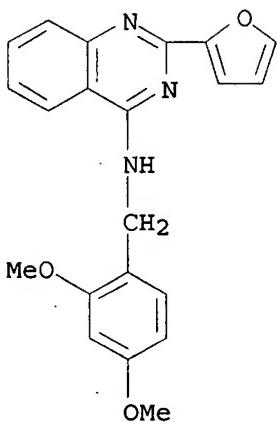
RN 896726-65-1 ZCPLUS

CN 4-Quinazolinamine, N-[(3,4-dimethoxyphenyl)methyl]-2-(2-furanyl)- (9CI)
(CA INDEX NAME)



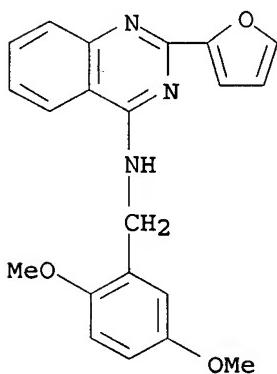
RN 896726-66-2 ZCPLUS

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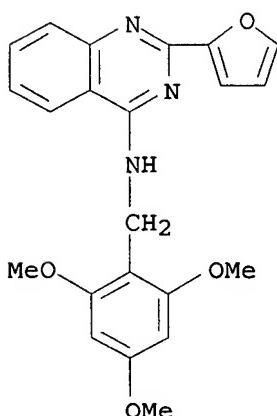
RN 896726-67-3 ZCPLUS

CN 4-Quinazolinamine, N-[(2,5-dimethoxyphenyl)methyl]-2-(2-furanyl)- (9CI)
(CA INDEX NAME)



RN 896726-68-4 ZCPLUS

CN 4-Quinazolinamine, 2-(2-furanyl)-N-[(2,4,6-trimethoxyphenyl)methyl]- (9CI)
(CA INDEX NAME)

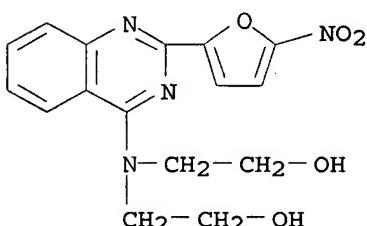


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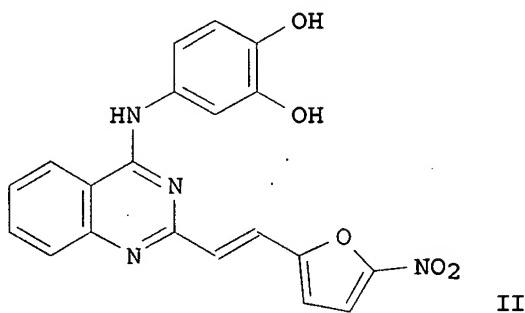
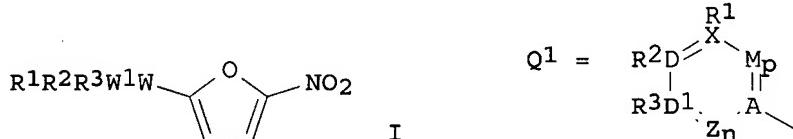
THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2006:405003 ZCPLUS
 DOCUMENT NUMBER: 146:155278
 TITLE: Non-stochastic and stochastic linear indices of the molecular pseudograph's atom-adjacency matrix: a novel approach for computational *in silico* screening and "rational" selection of new lead antibacterial agents
 AUTHOR(S): Marrero-Ponce, Yovani; Marrero, Ricardo Medina; Torrens, Francisco; Martinez, Yamile; Bernal, Milagros Garcia; Zaldivar, Vicente Romero; Castro, Eduardo A.; Abalo, Ricardo Grau
 CORPORATE SOURCE: Department of Pharmacy, Faculty of Chemical-Pharmacy, Central University of Las Villas, Santa Clara, 54830, Cuba
 SOURCE: Journal of Molecular Modeling (2006), 12(3), 255-271
 CODEN: JMMOKF; ISSN: 0948-5023
 URL: <http://www.springerlink.com/media/ef6tmfk36j3ttmb97w1h/contributions/1/2/v/4/l2v47qr26320v870.pdf>
 PUBLISHER: Springer GmbH
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 AB A novel approach (TOMOCOMD-CARDD) to computer-aided rational drug design is illustrated. This approach is based on the calcn. of the non-stochastic and stochastic linear indexes of the mol. pseudograph's atom-adjacency matrix representing mol. structures. These TOMOCOMD-CARDD descriptors are introduced for the computational (virtual) screening and rational selection of new lead antibacterial agents using linear discrimination anal. The two structure-based antibacterial-activity classification models, including non-stochastic and stochastic indexes, classify correctly 91.61% and 90.75%, resp., of 1525 chems. in training sets. These models show high Matthews correlation coeffs. (MCC = 0.84 and 0.82). An external validation process was carried out to assess the robustness and predictive power of the model obtained. These QSAR models permit the correct classification of 91.49% and 89.31% of 505 compds. in an external test set, yielding MCCs of 0.84 and 0.79, resp. The TOMOCOMD-CARDD approach compares satisfactorily with respect to nine of the most useful models for antimicrobial selection reported to date. Finally, an *in silico* screening of 87 new chems. reported in the antiinfective field with antibacterial activities is developed showing the ability of the TOMOCOMD-CARDD models to identify new lead antibacterial compds.
 IT 5055-20-9, Nifurquinazol
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (novel QSAR model TOMOCOMD-CARDD in computer-aided rational drug design for selection of new lead antibacterial agents using linear discrimination anal.)
 RN 5055-20-9 ZCPLUS
 CN Ethanol, 2,2'-[[2-(5-nitro-2-furanyl)-4-quinazolinyl]imino]bis- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2006:298831 ZCPLUS
 DOCUMENT NUMBER: 144:350707
 TITLE: Preparation of nitrofurans as antibacterials.
 INVENTOR(S): Chamberland, Suzanne; Malouin, Francois
 PATENT ASSIGNEE(S): Ulysses Pharmaceutical Products Inc., Can.
 SOURCE: PCT Int. Appl., 82 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|-------------------|-----------------|------------|
| WO 2006032138 | A1 | 20060330 | WO 2005-CA1436 | 20050922 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,
NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG,
SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,
YU, ZA, ZM, ZW | | | | |
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IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
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GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM | | | | |
| PRIORITY APPLN. INFO.: | | | US 2004-612148P | P 20040923 |
| OTHER SOURCE(S): | | MARPAT 144:350707 | | |
| GI | | | | |



AB Title compds. (I; W = null, CH:CH, N:CH; W1 = null, or together with R1, R2, R3 = Q1; D, D1, X, M, A, Z = CH, C, O, S, NH, N; n, p = 0-2; R1-R3 = null, H, OH, halo, Me, alkyl, alkenyl, alkynyl, alkoxy, alkenyloxy, alkynyloxy, aryl, CF3, PhO, etc.; with provisos), were prepared. Thus, title compound (II) (preparation outlined) showed a min. inhibitory concentration of 0.5

μg/mL against E. coli ATCC 25922.

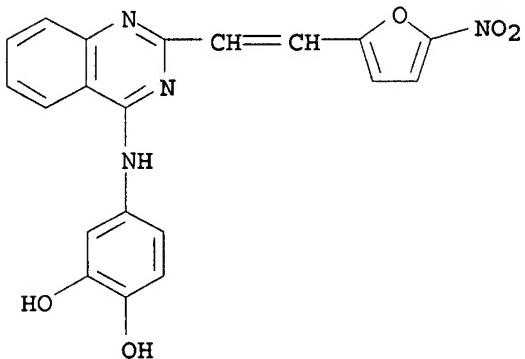
IT 881169-49-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitrofurans as antibacterials)

RN 881169-49-9 ZCPLUS

CN 1,2-Benzenediol, 4-[[2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:100738 ZCPLUS

DOCUMENT NUMBER: 144:198849

TITLE: Novel dosage form comprising modified-release and immediate-release active ingredients

INVENTOR(S): Vaya, Navin; Karan, Rajesh Singh; Sadanand, Sunil; Gupta, Vinod Kumar

PATENT ASSIGNEE(S): India

SOURCE: U.S. Pat. Appl. Publ., 49 pp., Cont.-in-part of U.S. Ser. No. 630,446.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 2006024365 | A1 | 20060202 | US 2005-134633 | 20050519 |
| IN 2002MU00697 | A | 20040529 | IN 2002-MU697 | 20020805 |
| IN 193042 | A1 | 20040626 | | |
| IN 2002MU00699 | A | 20040529 | IN 2002-MU699 | 20020805 |
| IN 2003MU00080 | A | 20050204 | IN 2003-MU80 | 20030122 |
| IN 2003MU00082 | A | 20050204 | IN 2003-MU82 | 20030122 |
| US 2004096499 | A1 | 20040520 | US 2003-630446 | 20030729 |
| PRIORITY APPLN. INFO.: | | | IN 2002-MU697 | A 20020805 |
| | | | IN 2002-MU699 | A 20020805 |
| | | | IN 2003-MU80 | A 20030122 |
| | | | IN 2003-MU82 | A 20030122 |
| | | | US 2003-630446 | A2 20030729 |

AB A dosage form comprising of a high dose, high solubility active ingredient as modified release and a low dose active ingredient as immediate release where the weight ratio of immediate release active ingredient and modified release active ingredient is from 1:10 to 1:15000 and the weight of modified

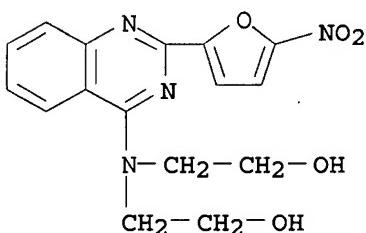
release active ingredient per unit is from 500 mg to 1500 mg; a process for preparing the dosage form. Tablets containing 10 mg sodium pravastatin and 1000 mg niacin were prepared. The release of sodium pravastatin after 24 h was 67.7%, and the release of niacin after 1 h was 84.1%.

IT 5055-20-9, Nifurquinazol

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel dosage form comprising modified-release and immediate-release active ingredients)

RN 5055-20-9 ZCPLUS

CN Ethanol, 2,2'-[[2-(5-nitro-2-furanyl)-4-quinazolinyl]imino]bis- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:686350 ZCPLUS

DOCUMENT NUMBER: 144:124809

TITLE: Identification of antimicrobial compounds active against intracellular *Staphylococcus aureus*

AUTHOR(S): Malouin, Francois; Brouillette, Eric; Martinez, Alejandro; Boyll, Bobbi J.; Toth, James L.; Gage, Jennifer L.; Allen, Norris E.

CORPORATE SOURCE: Faculte des Sciences, Centre d'Etude et de Valorisation de la Diversite Microbienne (CEVDM), Departement de Biologie, Universite de Sherbrooke, Sherbrooke, QC, J1K 2R1, Can.

SOURCE: FEMS Immunology and Medical Microbiology (2005), 45(2), 245-252

CODEN: FIMIEV; ISSN: 0928-8244

PUBLISHER: Elsevier B.V.

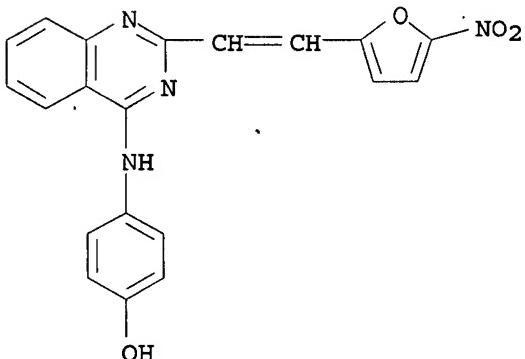
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Small-colony variants (SCVs) of *Staphylococcus aureus* exhibit characteristics of bacteria that can penetrate mammalian cells and remain intracellular and innocuous for indefinite periods. These properties make SCVs a convenient tool that can be used to identify new antibacterial agents having activity against intracellular, quiescent bacteria. Agents active against SCVs could be useful in the treatment of chronic staphylococcal infections such as bovine mastitis. An hemB deletion mutant of *S. aureus* Newbould, a bovine mastitis isolate, having a stable, genetically defined SCV phenotype, was used in a screening program to identify compds. active against intracellular, gram-pos. bacteria. Out of more than 260,000 compds. screened, 9 compds. having the desired properties were identified. The range of MICs against gram-pos. bacteria was \leq 0.12-32 μ g ml⁻¹. One of the compds. (number 8) showed excellent activity against gram-pos. (MICs \leq 0.12 μ g ml⁻¹) and gram-neg. (MICs \leq 0.12-4 μ g ml⁻¹) bacteria. Each of the nine compds. demonstrated efficacy in a neutropenic mouse thigh infection model. Two compds., including compound number 8, reduced nos. of bacteria in a mouse mastitis model of infection. Application of a stepwise screening process has identified lead compds. that may be useful for treating persistent, intracellular infections.

IT 60452-41-7

RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (antimicrobial screening against intracellular *Staphylococcus aureus*)
 RN 60452-41-7 ZCPLUS
 CN Phenol, 4-[[2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]amino]- (9CI)
 (CA INDEX NAME)



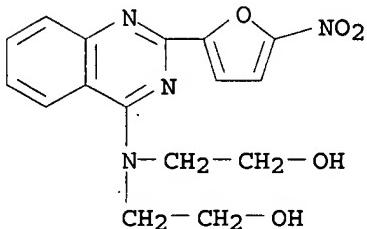
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:244333 ZCPLUS
 DOCUMENT NUMBER: 143:307
 TITLE: Atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints: a promising approach for modeling of antibacterial activity
 Marrero-Ponce, Yovani; Medina-Marrero, Ricardo; Torrens, Francisco; Martinez, Yamile; Romero-Zaldivar, Vicente; Castro, Eduardo A.
 AUTHOR(S):
 CORPORATE SOURCE: Department of Pharmacy, Faculty of Chemical-Pharmacy, Central University of Las Villas, Santa Clara, 54830, Cuba
 SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(8), 2881-2899
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The Topol. Mol. Computer Design (TOMOCOMD-CARDD) approach has been introduced for the classification and design of antimicrobial agents using computer-aided mol. design. For this propose, atom, atom-type, and total quadratic indexes have been generalized to codify chemical structure information. In this sense, stochastic quadratic indexes have been introduced for the description of the mol. structure. These stochastic fingerprints are based on a simple model for the intramol. movement of all valence-bond electrons. In this work, a complete data set containing 1006 antimicrobial agents is collected and presented. Two structure-based antibacterial activity classification models have been generated. The models (including nonstochastic and stochastic indexes) classify correctly more than 90% of 1525 compds. in training sets. These models permit the correct classification of 92.28% and 89.31% of 505 compds. in an external test sets. The approach, also, satisfactorily compares with respect to nine of the most useful models for antimicrobial selection reported to date. Finally, a virtual screening of 87 new compds. reported in the anti-infective field with antibacterial activities is developed showing the ability of the models to identify new leads as antibacterial.
 IT 5055-20-9, Nifurquinazol

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints as promising approach for modeling antibacterial activity)

RN 5055-20-9 ZCPLUS

CN Ethanol, 2,2'--[[2-(5-nitro-2-furanyl)-4-quinazolinyl]imino]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 91 THERE ARE 91 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:141062 ZCPLUS

DOCUMENT NUMBER: 142:240454

TITLE: Preparation of halogenated quinazolinyl nitrofurans as antibacterial agents

INVENTOR(S): Chamberland, Suzanne; Malouin, Francois

PATENT ASSIGNEE(S): Ulysses Pharmaceutical Products Inc., Can.

SOURCE: PCT Int. Appl., 59 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

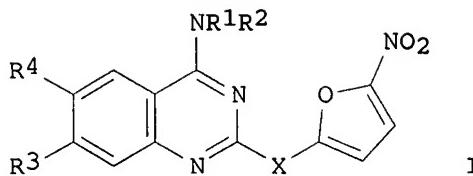
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|--|----------|------------------|------------|
| WO 2005014585 | A1 | 20050217 | WO 2004-CA1466 | 20040806 |
| WO 2005014585 | A8 | 20050909 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2004262533 | A1 | 20050217 | AU 2004-262533 | 20040806 |
| CA 2534405 | A1 | 20050217 | CA 2004-2534405 | 20040806 |
| EP 1660486 | A1 | 20060531 | EP 2004-761630 | 20040806 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK | | | | |
| CN 1832941 | A | 20060913 | CN 2004-80022816 | 20040806 |
| BR 2004013372 | A | 20061017 | BR 2004-13372 | 20040806 |
| JP 2007501809 | T | 20070201 | JP 2006-522859 | 20040806 |
| US 2006258693 | A1 | 20061116 | US 2006-567660 | 20060208 |
| PRIORITY APPLN. INFO.: | | | US 2003-493336P | P 20030808 |
| | | | WO 2004-CA1466 | W 20040806 |
| OTHER SOURCE(S): | CASREACT 142:240454; MARPAT 142:240454 | | | |

PL/PWB

GI



AB Title compds. [I; X = null, trans- or cis CH:CH; R1 = (hydroxy-substituted) alkyl, alkenyl, alkynyl, aryl; R2 = H, alkyl, aryl; R3, R4 = H, halo, solubilizing group; ≥ 1 of R3, R4 = halo], were prepared. Thus, p-aminophenol and 6-fluoro-2-[2-(5-nitro-2-furyl)vinyl]-4-chloroquinazoline (preparation given) were heated together in DMF for 2 h at 70-90° to give 6-fluoro-2-[2-(5-nitro-2-furyl)vinyl]-4-(p-hydroxyanilino)quinazoline. The latter showed a min. inhibitory concentration

of

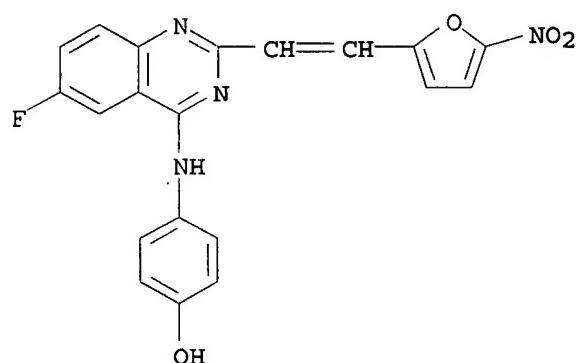
0.03-0.06 μ g/mL against. S. aureus ATCC 29213.

IT 844692-03-1P 844692-04-2P

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of halogenated quinazolinyl nitrofurans as antibacterial agents)

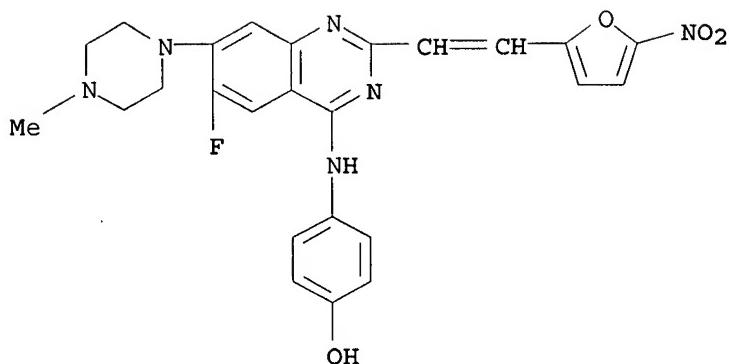
RN 844692-03-1 ZCPLUS

CN Phenol, 4-[[6-fluoro-2-[2-(5-nitro-2-furyl)ethenyl]-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



RN 844692-04-2 ZCPLUS

CN Phenol, 4-[[6-fluoro-7-(4-methyl-1-piperazinyl)-2-[2-(5-nitro-2-furyl)ethenyl]-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

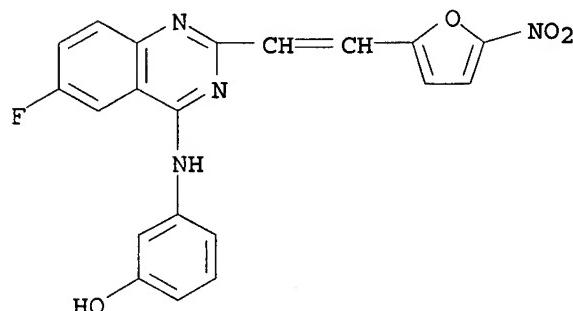


IT 844692-09-7P 844692-10-0P

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of halogenated quinazolinyl nitrofurans as antibacterial agents)

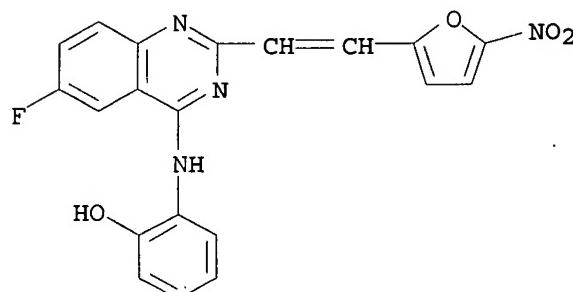
RN 844692-09-7 ZCPLUS

CN Phenol, 3-[[6-fluoro-2-[(2E)-2-(5-nitrofuran-2-yl)ethyl]amino]-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



RN 844692-10-0 ZCPLUS

CN Phenol, 2-[[6-fluoro-2-[(2E)-2-(5-nitrofuran-2-yl)ethyl]amino]-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

6

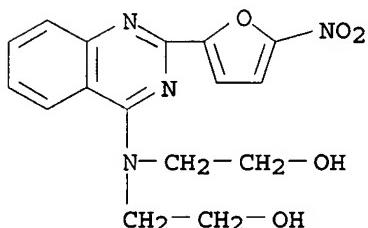
THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/ 567,660

ACCESSION NUMBER: 2004:550533 ZCPLUS
DOCUMENT NUMBER: 141:82297
TITLE: Immunostimulatory nucleic acids for the treatment of disorders associated with microorganisms, for preventing antibiotic resistance and for treating and preventing warts
INVENTOR(S): Bratzler, Robert L.; Petersen, Deanna M.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 54 pp., Cont. of U.S. Ser. No. 801,839, abandoned.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 2004131628 | A1 | 20040708 | US 2003-666733 | 20030919 |
| PRIORITY APPLN. INFO.: | | | US 2000-187834P | P 20000308 |
| | | | US 2001-801839 | B1 20010308 |

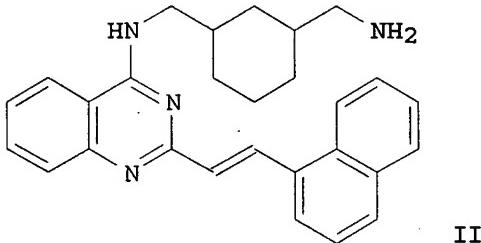
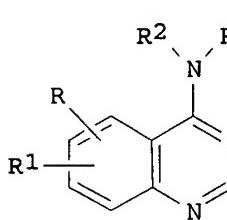
OTHER SOURCE(S): MARPAT 141:82297
AB The invention involves administration of an immunostimulatory nucleic acid alone or in combination with an antimicrobial agent for the treatment or prevention of infectious disease associated with microorganisms in subjects, for preventing antibiotic resistance and for treating and preventing warts. The combination of drugs are administered in synergistic amts. or in various dosages or at various time schedules. The invention also relates to kits and compns. concerning the combination of drugs.
IT 5055-20-9, Nifurquinazol
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(immunostimulatory nucleic acids for treatment of disorders associated with microorganisms, preventing antibiotic resistance, and treating and preventing warts, and use with other agents)
RN 5055-20-9 ZCPLUS
CN Ethanol, 2,2'-[[2-(5-nitro-2-furanyl)-4-quinazolinyl]imino]bis- (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:310971 ZCPLUS
DOCUMENT NUMBER: 140:321378
TITLE: Preparation of aminoquinazoline protein kinase B inhibitors as anticancer agents
INVENTOR(S): Barnickel, Gerhard; Eggenweiler, Hans-Michael;
Eiermann, Volker; Gericke, Rolf; Rautenberg, Wilfried;
Sirrenberg, Christian; Scharm, Burkhard
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

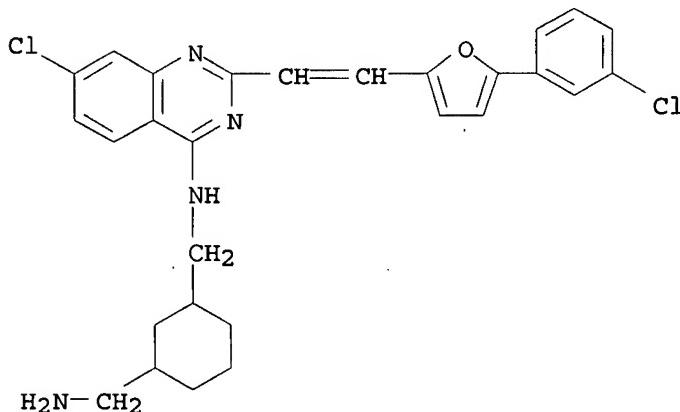
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|--|----------|-----------------|------------|
| WO 2004030671 | A2 | 20040415 | WO 2003-EP9391 | 20030825 |
| WO 2004030671 | A3 | 20040610 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2003258662 | A1 | 20040423 | AU 2003-258662 | 20030825 |
| PRIORITY APPLN. INFO.: | | | EP 2002-22152 | A 20021002 |
| | | | WO 2003-EP9391 | W 20030825 |
| OTHER SOURCE(S): GI | CASREACT 140:321378; MARPAT 140:321378 | | | |



- AB Title compds. I [wherein R and R1 = independently H, alkyl, OH, alkoxy, halo, N(R5)2, NO2, CN, CHO, alkanoyl, CON(R5)2, CO2R5, allyl, CH=CHCO2R5, CH=CHCON(R5)2, alkylsulfonyl, or (un)substituted Ph; R2 and R3 = independently H, (cyclo)alkyl, (un)substituted heterocyclyl(alkyl), alkoxy(alkyl), amino(alkyl), aryl(alkyl), etc.; or NR2R3 = (un)substituted heterocyclyl; R4 = (un)substituted Ph, naphthyl, biphenyl, or heterocyclyl; R5 = H or alkyl; Y = a direct bond, (CH2)n, or NR5(CH2)m; m = 0-6; n = 1-6; and pharmaceutically tolerable salts and solvates thereof] were prepared via solution and solid-phase methods as protein kinase B (PKB or Akt or RAC) inhibitors (no data). For example, cyclization of anthranilic acid with acetic anhydride gave the benzoxazinone, which was treated with ammonium acetate in DMF to afford 2-methylquinazolin-4-one (no data). Condensation with naphthalene-1-carbaldehyde in AcOH to provide the vinyl derivative, followed by chlorination and coupling with [(3-aminomethylcyclohexyl)methyl]amine, gave II. Also claimed is the use of I and their pharmaceutical compns. for the treatment of hyperproliferative disorders, such as cancer, psoriasis, arthritis, inflammation, endometriosis, scarring, or benign prostatic hyperplasia (no data).
- IT 406207-06-5P, [(3-Aminomethylcyclohexyl)methyl][7-chloro-2-[2-[5-(3-chlorophenyl)furan-2-yl]vinyl]quinazolin-4-yl]amine
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (PKB inhibitor; preparation of aminoquinazoline PKB inhibitors as anticancer agents)
- RN 406207-06-5 ZCPLUS

10/ 567,660

CN 1,3-Cyclohexanedimethanamine, N-[7-chloro-2-[2-[5-(3-chlorophenyl)-2-furanyl]ethenyl]-4-quinazolinyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 10 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:205966 ZCPLUS

DOCUMENT NUMBER: 142:197901

TITLE: Product class 13: quinazolines

AUTHOR(S): Kikelj, D.

CORPORATE SOURCE: Germany

SOURCE: Science of Synthesis (2004), 16, 573-749

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

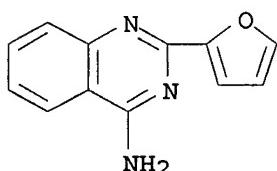
AB A review. Preparation of quinazolines by ring closure and ring transformation reactions as well as aromatization and substituent modification is given.

IT 40172-85-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of quinazolines)

RN 40172-85-8 ZCPLUS

CN 4-Quinazolinamine, 2-(2-furanyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1014 THERE ARE 1014 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:146768 ZCPLUS

DOCUMENT NUMBER: 140:350028

TITLE: Designing Antibacterial Compounds through a Topological Substructural Approach

AUTHOR(S): Molina, Enrique; Gonzales Diaz, Humberto; Gonzalez, Maykel Perez; Rodriguez, Elismary; Uriarte, Eugenio

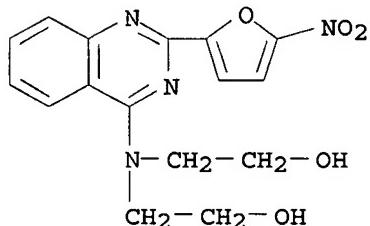
CORPORATE SOURCE: Department of Chemistry and Pharmacy Faculty of Engineering Chemistry and Pharmacy, University of

SOURCE: Camaguey, Camaguey, 74650, Cuba
 Journal of Chemical Information and Computer Sciences
 (2004), 44(2), 515-521
 CODEN: JCISD8; ISSN: 0095-2338

PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A novel application of TOPol. Substructural Mol. DEsign (TOPS-MODE) was carried out in antibacterial drugs using computer-aided mol. design. Two series of compds., one containing antibacterial and the other containing non-antibacterial compds., were processed by a k-means cluster anal. in order to design training and predicting series. All clusters had a p-level < 0.005. Afterward, a linear classification function has been derived toward discrimination between antibacterial and non-antibacterial compds. The model correctly classifies 94% of active and 86% of inactive compds. in the training series. More specifically, the model showed a global good classification of 91%, i.e., 263 cases out of 289. In predicting series, the model has shown overall predictabilities of 91 and 83% for active and inactive compds., resp. Thereby, the model has a global percentage of good classification of 89%. The TOPS-MODE approach, also, similarly compares with respect to one of the most useful models for antimicrobials selection reported to date.

IT 5055-20-9, Nifurquinazol
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (designing antibacterial compds. through a topol. substructural approach)
 RN 5055-20-9 ZCPLUS
 CN Ethanol, 2,2'-[{[2-(5-nitro-2-furanyl)-4-quinazolinyl]imino}bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:41226 ZCPLUS
 DOCUMENT NUMBER: 140:105321
 TITLE: Methods and compositions relating to isoleucine boroproline compounds
 INVENTOR(S): Adams, Sharlene; Miller, Glenn T.; Jesson, Michael I.; Jones, Barry
 PATENT ASSIGNEE(S): Point Therapeutics, Inc., USA
 SOURCE: PCT Int. Appl., 152 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|------|----------|-----------------|----------|
| WO 2004004658 | A2 | 20040115 | WO 2003-US21405 | 20030709 |

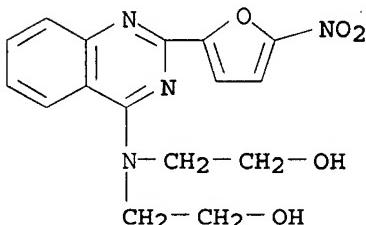
| | | | | |
|------------------------|--|----------|-----------------|------------|
| WO 2004004658 | A3 | 20050804 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZW | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| CA 2491466 | A1 | 20040115 | CA 2003-2491466 | 20030709 |
| AU 2003265264 | A1 | 20040123 | AU 2003-265264 | 20030709 |
| US 2004077601 | A1 | 20040422 | US 2003-616694 | 20030709 |
| US 2005084490 | A1 | 20050421 | US 2003-616409 | 20030709 |
| EP 1578434 | A2 | 20050928 | EP 2003-763380 | 20030709 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | |
| JP 2006507352 | T | 20060302 | JP 2004-562634 | 20030709 |
| CN 1802090 | A | 20060712 | CN 2003-821282 | 20030709 |
| CN 1826129 | A | 20060830 | CN 2003-821281 | 20030709 |
| IN 2005KN00151 | A | 20050916 | IN 2005-KN151 | 20050208 |
| PRIORITY APPLN. INFO.: | | | US 2002-394856P | P 20020709 |
| | | | US 2002-414978P | P 20021001 |
| | | | US 2003-466435P | P 20030428 |
| | | | WO 2003-US21405 | W 20030709 |

OTHER SOURCE(S): MARPAT 140:105321

AB A method for treating subjects with, inter alia, abnormal cell proliferation or infectious disease using agents of formula (I, AmNHCH(CH(CH₃)CH₂CH₃)COA1R) (where Am and A1 are amino acids and R = organo boronates, organo phosphonates, fluoroalkyl ketones, alphaketos, N-peptioly1-O-(acylhydroxylamines), azapeptides, azetidines, fluoroolefins dipeptide isosteres, peptidyl (α -aminoalkyl) phosphonate esters, aminoacyl pyrrolidine-2-nitriles and 4-cyanothiazolidides) is claimed. Methods for stimulating an immune response using the compds. of the invention are also claimed. Compns. containing Ile-boroPro compds. are also provided as are kits containing the compns. The invention embraces the use of these compds. alone or in combination with other therapeutic agents.

IT 5055-20-9, Nifurquinazol
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (therapeutic methods and compns. relating to isoleucine boroproline compds. alone or in combination with other drugs, antibodies, or antigens)

RN 5055-20-9 ZCAPLUS
 CN Ethanol, 2,2'-[[2-(5-nitro-2-furanyl)-4-quinazolinyl]imino]bis- (9CI) (CA INDEX NAME)



TITLE: Preparation of (indazol-5-ylamino)quinazolines as Rho-kinase inhibitors
 INVENTOR(S): Nagarathnam, Dhanapalan; Asgari, Davoud; Shao, Jianxing; Liu, Xiao-Gao; Khire, Uday; Wang, Chunguang; Hart, Barry; Boyer, Stephen; Weber, Olaf; Lynch, Mark; Bankston, Donald
 PATENT ASSIGNEE(S): Bayer Corporation, USA
 SOURCE: PCT Int. Appl., 74 pp.
 CODEN: PIIXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|------------------|------------|
| WO 2002076976 | A2 | 20021003 | WO 2002-US8659 | 20020322 |
| WO 2002076976 | A3 | 20021212 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2441492 | A1 | 20021003 | CA 2002-2441492 | 20020322 |
| AU 2002250394 | A1 | 20021008 | AU 2002-250394 | 20020322 |
| US 2003125344 | A1 | 20030703 | US 2002-103566 | 20020322 |
| EP 1370553 | A2 | 20031217 | EP 2002-719303 | 20020322 |
| EP 1370553 | B1 | 20060510 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| JP 2004524350 | T | 20040812 | JP 2002-576234 | 20020322 |
| AT 325795 | T | 20060615 | AT 2002-719303 | 20020322 |
| TW 261055 | B | 20060901 | TW 2002-91105591 | 20020322 |
| PT 1370553 | T | 20060929 | PT 2002-719303 | 20020322 |
| ES 2264477 | T3 | 20070101 | ES 2002-2719303 | 20020322 |
| US 2003220357 | A1 | 20031127 | US 2002-252369 | 20020924 |
| CA 2507381 | A1 | 20040408 | CA 2003-2507381 | 20030924 |
| WO 2004029045 | A2 | 20040408 | WO 2003-US29538 | 20030924 |
| WO 2004029045 | A3 | 20040722 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2003270785 | A1 | 20040419 | AU 2003-270785 | 20030924 |
| EP 1542992 | A2 | 20050622 | EP 2003-752497 | 20030924 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| JP 2006508068 | T | 20060309 | JP 2004-540124 | 20030924 |
| HK 1061030 | A1 | 20060908 | HK 2004-104115 | 20040609 |
| US 2006142313 | A1 | 20060629 | US 2006-354977 | 20060216 |
| US 2006142314 | A1 | 20060629 | US 2006-354978 | 20060216 |
| PRIORITY APPLN. INFO.: | | | US 2001-277974P | P 20010323 |
| | | | US 2001-315341P | P 20010829 |

| | |
|-----------------|-------------|
| US 2001-315338P | P 20010829 |
| US 2002-103565 | B1 20020322 |
| US 2002-103566 | B1 20020322 |
| WO 2002-US8659 | W 20020322 |
| US 2002-252369 | A 20020924 |
| WO 2003-US29538 | W 20030924 |

OTHER SOURCE(S) : CASREACT 137:279208; MARPAT 137:279208

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

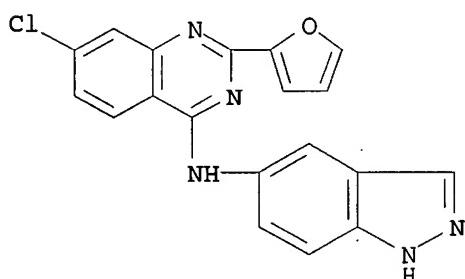
AB Title compds. I [Y = N, CR17; X = alkyl, alkoxy, thioalkoxy, amido, etc.; p = 0-3; a, c = CR5, NR6, etc.; b = CR5, N; A = H, halo, carboxy, cyano, alkoxy, etc.; B = (un)substituted up to 3 times in any position by R5; R1,6 = H, alkyl; R2-5 = H, alkyl, alkenyl; R17 = H, alkyl, CN with provisions] were prepared For instance, 2,4-Dichloroquinazoline (preparation given) was reacted with 5-aminoindazole (THF/H₂O, KOAc) to give 2-(N-(1H-indazol-5-yl)amino)-4-chloroquinazoline in 92% yield. This was coupled to 2,4-dichlorophenylboronic acid (ethylene glycol di-Me ether, Pd(dppf)Cl₂, NaHCO₃, reflux) to give II. I are rho-kinase inhibitors and are useful for inhibiting tumor growth, treating erectile dysfunction and coronary heart disease.

IT 461037-95-6P 461037-96-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (rho-kinase inhibitor; preparation of (indazol-5-ylamino)quinazolines as Rho-kinase inhibitors)

RN 461037-95-6 ZCPLUS

CN 4-Quinazolinamine, 7-chloro-2-(2-furanyl)-N-1H-indazol-5-yl- (9CI) (CA INDEX NAME)



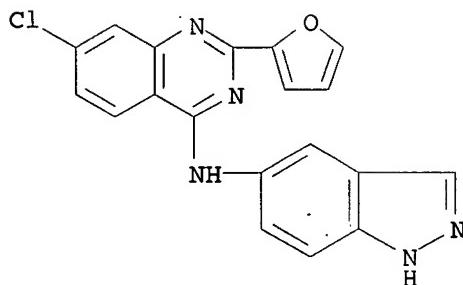
RN 461037-96-7 ZCPLUS

CN 4-Quinazolinamine, 7-chloro-2-(2-furanyl)-N-1H-indazol-5-yl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

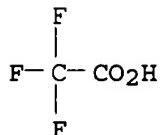
CM 1

CRN 461037-95-6

CMF C19 H12 Cl N5 O



CM 2

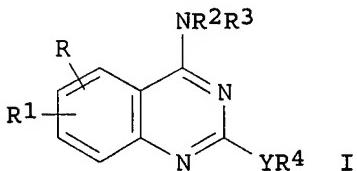
CRN 76-05-1
CMF C2 H F3 O2

L4 ANSWER 14 OF 40 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:240745 ZCAPLUS
 DOCUMENT NUMBER: 136:279467
 TITLE: Preparation of quinazolin-4-ylamines as glycoprotein IbIX antagonists.
 INVENTOR(S): Mederski, Werner; Devant, Ralf; Barnickel, Gerhard;
 Bernotat-Danielowski, Sabine; Vickers, James; Cezanne,
 Bertram; Dhanoa, Daljit; Zhao, Bao-Ping; Rinker,
 James; Player, Mark R.; Jaeger, Edward; Soll, Richard
 PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
 SOURCE: PCT Int. Appl., 90 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| WO 2002024666 | A2 | 20020328 | WO 2001-EP10704 | 20010917 |
| WO 2002024666 | A3 | 20020926 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
UZ, VN, YU, ZA, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2422560 | A1 | 20020328 | CA 2001-2422560 | 20010917 |
| AU 2002013923 | A5 | 20020402 | AU 2002-13923 | 20010917 |
| EP 1318985 | A2 | 20030618 | EP 2001-982300 | 20010917 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |

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|------------------------|-------------|-----------------|------------|
| BR 2001014021 | A 20030819 | BR 2001-14021 | 20010917 |
| HU 200302429 | A2 20031028 | HU 2003-2429 | 20010917 |
| JP 2004509875 | T 20040402 | JP 2002-529076 | 20010917 |
| NO 2003001267 | A 20030519 | NO 2003-1267 | 20030319 |
| US 2004044204 | A1 20040304 | US 2003-380909 | 20030320 |
| ZA 2003003069 | A 20040719 | ZA 2003-3069 | 20030417 |
| PRIORITY APPLN. INFO.: | | US 2000-666117 | A 20000920 |
| | | WO 2001-EP10704 | W 20010917 |

OTHER SOURCE(S) : MARPAT 136:279467
GI



AB Title compds. [I; R, R1 = H, alkyl, halo, amino, NO₂, cyano, allyl, (substituted) Ph, etc.; R₂, R₃ = H, alkyl, cycloalkyl, (substituted) heterocyclyl, hydroxyalkyl, etc.; NR₂R₃ = (substituted) heterocyclyl; R₄ = (substituted) aryl, heterocyclyl; Y = (CH:CH)_n; n = 1, 2; with provisos], were prepared for treatment of thrombotic disorders (no data). Thus, 4-chloro-2-(2-naphthalen-1-ylvinyl)quinazoline and 1,3-bis(aminomethyl)cyclohexane were heated in EtOH at 80° for 3 h to give 4-[N-(3-aminomethylcyclohexylmethyl)amino]-2-(2-naphthalen-1-ylvinyl)quinazoline.

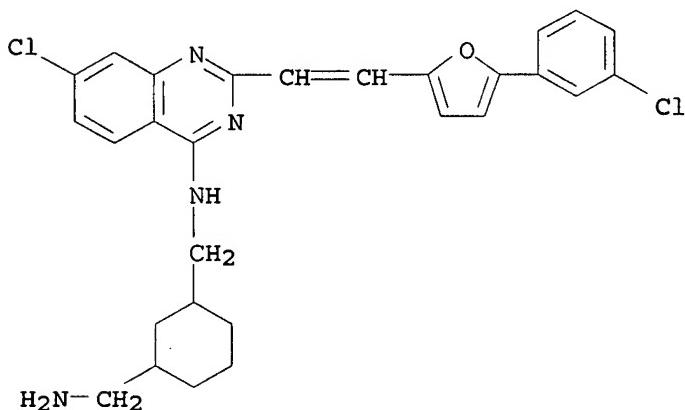
IT 406207-06-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

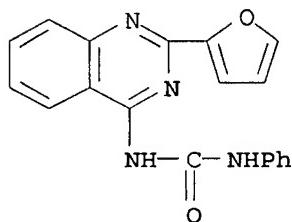
(preparation of quinazolin-4-ylamines as glycoprotein IbIX antagonists)

RN 406207-06-5 ZCPLUS

CN 1,3-Cyclohexanedimethanamine, N-[7-chloro-2-[2-[5-(3-chlorophenyl)-2-furanyl]ethenyl]-4-quinazolinyl]- (9CI) (CA INDEX NAME)



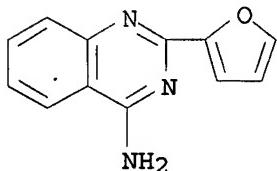
TITLE: Isoquinoline and Quinazoline Urea Analogues as Antagonists for the Human Adenosine A3 Receptor
 AUTHOR(S): Van Muijlwijk-Koezen, Jacqueline E.; Timmerman, Henk; Van der Goot, Henk; Menge, Wiro M. P. B.; Von Kuenzel, Jacobien Frijtag; De Groote, Miriam; IJzerman, Adriaan P.
 CORPORATE SOURCE: Leiden/Amsterdam Center for Drug Research Division of Medicinal Chemistry Department of Pharmacochemistry, Vrije Universiteit, Amsterdam, 1081 HV, Neth.
 SOURCE: Journal of Medicinal Chemistry (2000), 43(11), 2227-2238
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Isoquinoline and quinazoline urea derivs. were found to bind to human adenosine A3 receptors. Series of N-phenyl-N'-quinazolin-4-ylurea derivs. and N-phenyl-N'-isoquinolin-1-ylurea derivs. were synthesized and tested in radioligand binding assays on their adenosine receptor affinities. A structure-affinity anal. indicated that on the 2-position of the quinazoline ring or the equivalent 3-position of the isoquinoline ring a Ph or heteroaryl substituent increased the adenosine A3 receptor affinity in comparison to unsubstituted or aliphatic derivs. Furthermore, the structure-affinity relationship of substituted phenylurea analogs was investigated. Substituents such as electron-withdrawing or electron-donating groups were introduced at different positions of the benzene ring to probe electronic and positional effects of substitution. Substitution on the 3- or 4-position of the Ph ring decreased the adenosine A3 receptor affinity. Substitution at position 2 with an electron-donating substituent, such as Me or methoxy, increased human adenosine A3 receptor affinity, whereas substitution on the 2-position with an electron-withdrawing substituent did not influence affinity. Combination of the optimal substituents in the two series had an additive effect, which led to the potent human adenosine A3 receptor antagonist N-(2-methoxyphenyl)-N'-(2-(3-pyridyl)quinazolin-4-yl)urea (VUF5574, I) showing a Ki value of 4 nM and being at least 2500-fold selective vs. A1 and A2A receptors. Compound I competitively antagonized the effect of an agonist in a functional A3 receptor assay, i.e., inhibition of cAMP production in cells expressing the human adenosine A3 receptor; a pA₂ value of 8.1 was derived from a Schild plot. In conclusion, compound I is a potent and selective human adenosine A3 receptor antagonist and might be a useful tool in further characterization of the human A3 receptor.
 IT 280139-00-6P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation of isoquinoline and quinazoline urea analogs as antagonists for human adenosine A3 receptor)
 RN 280139-00-6 ZCAPLUS
 CN Urea, N-[2-(2-furanyl)-4-quinazolinyl]-N'-phenyl- (9CI) (CA INDEX NAME)



RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoquinoline and quinazoline urea analogs as antagonists for human adenosine A₃ receptor)

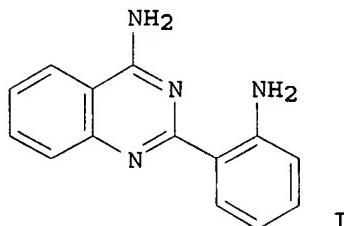
RN 40172-85-8 ZCPLUS

CN 4-Quinazolinamine, 2-(2-furanyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:248619 ZCPLUS
DOCUMENT NUMBER: 133:30698
TITLE: Microwave-enhanced synthesis of 4-aminoquinazolines
AUTHOR(S): Seijas, Julio A.; Vazquez-Tato, M. Pilar; Martinez, M.
Montserrat
CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de
Ciencias, Universidad de Santiago de Compostela, Lugo,
27080, Spain
SOURCE: Tetrahedron Letters (2000), 41(13), 2215-2217
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:30698
GI



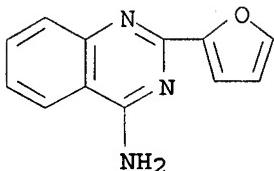
AB Aromatic nitriles react with anthranilonitrile in a domestic microwave oven to afford good yields of the corresponding 4-aminoquinazolines, e.g. I, in a very short irradiation time.

IT 40172-85-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(microwave enhanced preparation of aminoquinazolines)

RN 40172-85-8 ZCAPLUS

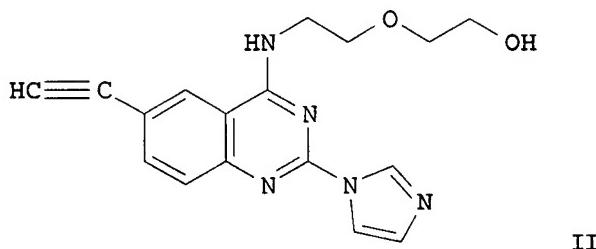
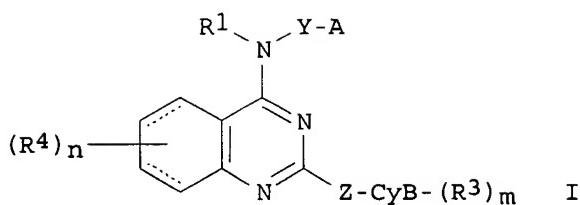
CN 4-Quinazolinamine, 2-(2-furanyl)- (9CI) (CA INDEX NAME)



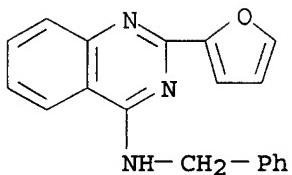
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 40 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1995:795361 ZCAPLUS
 DOCUMENT NUMBER: 124:29779
 TITLE: 4-Aminoquinazoline derivatives as inhibitors of cGMP phosphodiesterase and TXA2 synthetase
 INVENTOR(S): Lee, Sung J.; Konishi, Yoshitaka; Macina, Orest T.; Kondo, Kigen; Yu, Dingwei T.
 PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
 SOURCE: U.S., 42 pp. Cont.-in-part of U.S. Ser. No. 76,431, abandoned.
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|-----------|-----------------|-------------|
| US 5439895 | A | 19950808 | US 1993-154691 | 19931119 |
| JP 06192235 | A | 19940712 | JP 1993-197039 | 19930714 |
| CA 2100626 | A1 | 19940116 | CA 1993-2100626 | 19930715 |
| KR 191416 | B1 | 19990615 | KR 1993-13549 | 19930715 |
| AT 208771 | T | 20011115 | AT 1993-305557 | 19930715 |
| ES 2167325 | T3 | 20020516 | ES 1993-305557 | 19930715 |
| PT 579496 | T | 20020531 | PT 1993-305557 | 19930715 |
| JP 08099962 | A | 19960416 | JP 1995-264667 | 19950920 |
| JP 2923742 | B2 | 19990726 | | |
| PRIORITY APPLN. INFO.: | | | US 1992-913473 | B2 19920715 |
| | | | US 1993-76431 | B2 19930614 |
| OTHER SOURCE(S): | MARPAT | 124:29779 | | |
| GI | | | | |

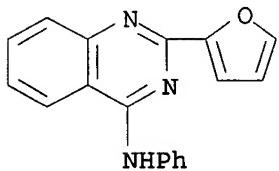


- AB** The compds. of the formula I and acid addition salts thereof, salts thereof, and hydrates thereof wherein R1 is hydrogen or C1-4 alkyl; Y is C1-6 alkylene; A is OR0 or S(O)pR0, in which R0 is C1-4 alkyl-hydroxy; p is 0-2; Z is single bond, methylene, ethylene, vinylene or ethynylene; CyB is (1) 7-membered, unsatd. or partially saturated, monocyclic hetero ring containing
as hetero atoms, one, two or three nitrogen atoms, (2) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms, two
or
three nitrogen atoms, (3) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atom, one nitrogen atom, (4) 4- or
5-membered, unsatd. or partially saturated, monocyclic hetero ring containing
as
hetero atoms, one, two or three nitrogen atoms, or (5) 4-7 membered,
unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms,
one or two oxygen atoms, or one or two sulfur atoms; R3 = e.g., H, C1-4
alkyl, C1-4 alkoxy; R4 = e.g., H, C1-4 alkyl, C1-4 alkoxy; and m and n
independently are 1 or 2; with the proviso that (1) a CyB ring does not
bond to Z through a nitrogen atom in the CyB ring when Z is vinylene or
ethynylene, have inhibitory effect on cGMP-PDE, and addnl. on TXA2
synthetase. Thus, e.g., 2-(1-imidazolyl)-4-[2-(2-
hydroxyethoxy)ethyl]amino-6-ethynylquinazoline.2HCl (II.2HCl) (prepared by
desilylation of a silylacetylene precursor) exhibited inhibitory effect on
cGMP-PDE and TXA2 synthetase with IC50 = 4.6 + 10-8 M and 1.33
+ 10-6 M, resp. Pharmaceutical formulations were given.
- IT** 157863-03-1P 157863-04-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(4-aminoquinazoline derivs. as inhibitors of cGMP phosphodiesterase and
TXA2 synthetase)
- RN** 157863-03-1 ZCAPLUS
CN 4-Quinazolinamine, 2-(2-furanyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 157863-04-2 ZCPLUS

CN 4-Quinazolinamine, 2-(2-furanyl)-N-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 18 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:761961 ZCPLUS

DOCUMENT NUMBER: 123:340173

TITLE: 4-Aminoquinazoline derivatives as inhibitors of cyclic guanosine 3',5'-monophosphate phosphodiesterase and thromboxane A₂ synthetase

INVENTOR(S): Lee, Sung J.; Konishi, Yoshitaka; Macina, Orest T.; Kondo, Kigen; Yu, Dingwei T.

PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan

SOURCE: U.S., 44 pp. Cont.-in-part of U.S. Ser. No. 76,431, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

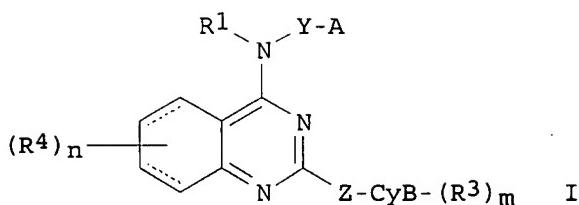
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| US 5436233 | A | 19950725 | US 1993-154518 | 19931119 |
| JP 06192235 | A | 19940712 | JP 1993-197039 | 19930714 |
| CA 2100626 | A1 | 19940116 | CA 1993-2100626 | 19930715 |
| KR 191416 | B1 | 19990615 | KR 1993-13549 | 19930715 |
| AT 208771 | T | 20011115 | AT 1993-305557 | 19930715 |
| ES 2167325 | T3 | 20020516 | ES 1993-305557 | 19930715 |
| PT 579496 | T | 20020531 | PT 1993-305557 | 19930715 |
| JP 08099962 | A | 19960416 | JP 1995-264667 | 19950920 |
| JP 2923742 | B2 | 19990726 | | |

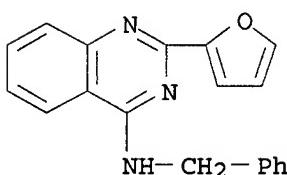
PRIORITY APPLN. INFO.: US 1992-913473 B2 19920715
US 1993-76431 B2 19930614OTHER SOURCE(S): CASREACT 123:340173; MARPAT 123:340173
GI



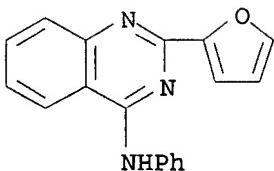
AB Title compds. I [R1 is H, C1-4 alkyl; Y is a single bond or C1-6 alkylene; A is (i) CyA-(R2)l, (ii) OR0 or S(O)pR0 in which R0 is ROA or ROB; ROA is CyA-(R2)l; ROB is H or C1-4 alkyl; p is 0-2; CyA is, e.g., (1) 3-7 membered, saturated or unsatd., monocyclic carbocyclic ring, (2) 7-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms,
one nitrogen atom, one nitrogen and one oxygen atoms, two nitrogen and one oxygen atoms, or one nitrogen and two oxygen atoms, (3) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms,
one nitrogen and one oxygen atoms, two nitrogen and one oxygen atoms, or one nitrogen and two oxygen atoms; R2 is R2A or R2B; R2A is, e.g., CF3, OCF3; R2B is, e.g., H, C1-4 alkyl, C1-4 alkoxy; Z is ZA or ZB, ZA is methylene, ethylene, vinylene, ethynylene; ZB is a single bond; CyB is, e.g., (1) 7-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms, one, two or three nitrogen atoms, (2) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms,
two or three nitrogen atoms, (3) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as a hetero atom, one nitrogen atom; R3 = e.g., H, C1-4 alkyl; R4 = e.g., NHSO2R11, R11 = e.g., C1-4 alkyl; l, m, n are independently 1 or 2 (with provisos)] are provided as inhibitors of cGMP-PDE and TXA2 synthetase. Thus, e.g., treatment of 2-(1-imidazolyl)-4-(2-methoxyethyl)amino-6-(2-triethylsilylethynyl)quinazoline (preparation given) with tetrabutylammonium fluoride afforded 6-ethynyl-4-(2-methoxyethyl)amino-2-(1-imidazolyl)quinazoline (II); II.2HCl demonstrated inhibition of cGMP-PDE with and TXA2 synthetase with IC50 = 4.6 + 10-8 and 2.4 + 10-6 M, resp. Pharmaceutical formulations were given.

IT 157863-03-1P 157863-04-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (4-aminoquinazoline derivs. as inhibitors of cyclic guanosine 3',5'-monophosphate phosphodiesterase and thromboxane A2 synthetase)

RN 157863-03-1 ZCAPLUS
CN 4-Quinazolinamine, 2-(2-furanyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 157863-04-2 ZCAPLUS
CN 4-Quinazolinamine, 2-(2-furanyl)-N-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 19 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:746792 ZCPLUS

DOCUMENT NUMBER: 123:132021

TITLE: Discovery of Potent Cyclic GMP Phosphodiesterase Inhibitors. 2-Pyridyl- and 2-Imidazolylquinazolines Possessing Cyclic GMP Phosphodiesterase and Thromboxane Synthesis Inhibitory Activities

AUTHOR(S): Lee, Sung J.; Konishi, Yoshitaka; Yu, Dingwei T.; Miskowski, Tamara A.; Riviello, Christopher M.; Macina, Orest T.; Frierson, Manton R.; Kondo, Kigen; Sugitani, Masafumi; et al.

CORPORATE SOURCE: Biofor Inc., Waverly, PA, 18471, USA

SOURCE: Journal of Medicinal Chemistry (1995), 38(18), 3547-57
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

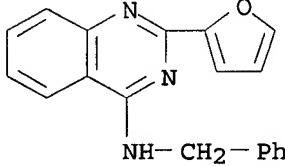
AB Moderate cyclic GMP phosphodiesterase (cGMP-PDE, PDE V) inhibitor 2-phenyl-4-anilinoquinazoline (I) was identified utilizing MultiCASE assisted drug design (MCADD) technol. Modification of I was conducted at the 2-, 4-, and 6-positions of the quinazoline ring for enhancement of cGMP-PDE inhibitory activity. The 6-substituted 2-(imidazol-1-yl)quinazolines are 1000 times more potent in in vitro PDE V enzyme assay than the well-known inhibitor zaprinast. The 6-substituted derivs. of 2-(3-pyridyl)quinazoline and 2-(imidazol-1-yl)quinazoline exhibited more than 1000-fold selectivity for PDE V over the other four PDE isoenzymes. In addition, 3 cGMP-PDE inhibitors were found to have an addnl. property of thromboxane synthesis inhibitory activity.

IT 157863-03-1P 157863-04-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(pyridyl- and imidazolylquinazolines as cyclic GMP phosphodiesterase and thromboxane synthesis inhibitors)

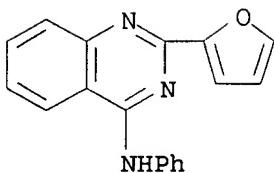
RN 157863-03-1 ZCPLUS

CN 4-Quinazolinamine, 2-(2-furanyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 157863-04-2 ZCPLUS

CN 4-Quinazolinamine, 2-(2-furanyl)-N-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 20 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:605373 ZCPLUS

DOCUMENT NUMBER: 121:205373

TITLE: 4-aminoquinazoline derivatives, and their use as medicine

INVENTOR(S): Lee, Sung Jai; Konishi, Yoshitaka; Macina, Orest Taras; Kondo, Kigen; Yu, Dingwei Tim

PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 86 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

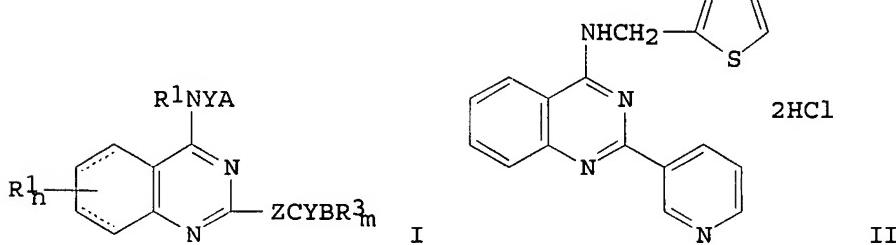
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| EP 579496 | A1 | 19940119 | EP 1993-305557 | 19930715 |
| EP 579496 | B1 | 20011114 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
| JP 06192235 | A | 19940712 | JP 1993-197039 | 19930714 |
| CA 2100626 | A1 | 19940116 | CA 1993-2100626 | 19930715 |
| KR 191416 | B1 | 19990615 | KR 1993-13549 | 19930715 |
| AT 208771 | T | 20011115 | AT 1993-305557 | 19930715 |
| ES 2167325 | T3 | 20020516 | ES 1993-305557 | 19930715 |
| PT 579496 | T | 20020531 | PT 1993-305557 | 19930715 |
| JP 08099962 | A | 19960416 | JP 1995-264667 | 19950920 |
| JP 2923742 | B2 | 19990726 | | |
| PRIORITY APPLN. INFO.: | | | US 1992-913473 | A 19920715 |
| | | | US 1993-76431 | A 19930614 |

OTHER SOURCE(S): MARPAT 121:205373

GI



AB The title compds. I wherein R1 is H or alkyl; Y is bond or alkylene; A is (i) -CyAR2, (ii) -OR0 or -S(O)pR0, R0 = H, alkyl, etc., p is 0-2, (iii) -NR16R17, R16, R17 are H, alkyl; CyA is (1) a 3-7 membered monocyclic carbocyclic ring, (2) a 4-7 membered monocyclic hetero ring containing as hetero atoms, one N atom, one N and one O atoms, two N and one O atoms, or one N and two O atoms, (3) a 4-7 membered monocyclic hetero ring containing as hetero atoms, 1 or 2 O or S atoms, R2 is (1) H, (2) alkyl, (3) alkoxy, (4)

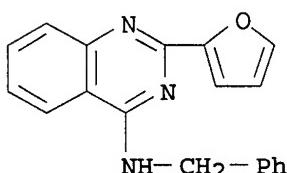
-COOR₅, in which R₅ is H or alkyl, (5) -NR₆R₇, R₆, R₇ are H, alkyl, (6) -SO₂NR₆R₇, (7) halogen, (8) CF₃, (9) NO₂ or (10) CF₃O; Z is bond, methylene, ethylene, vinylene or ethynylene; CyB is a heterocyclic ring; R₃ is H, alkyl, alkoxy, halogen or CF₃; R₄ is H, alkyl, alkoxy, etc., and acid addition salts thereof, salts thereof, and hydrates thereof were prepared and have inhibitory effect on cGMP-PDE, or addnl. on TXA₂ synthetase. Thus, a representative prepared compound II had inhibitory activity IC₅₀ of 3.6 x 10⁻⁷ on cGMP-PDE.

IT 157863-03-1P 157863-04-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as cardiovascular agents)

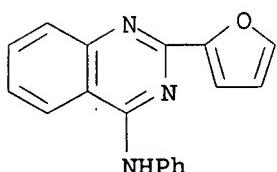
RN 157863-03-1 ZCPLUS

CN 4-Quinazolinamine, 2-(2-furanyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 157863-04-2 ZCPLUS

CN 4-Quinazolinamine, 2-(2-furanyl)-N-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 21 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:32975 ZCPLUS

DOCUMENT NUMBER: 106:32975

TITLE: 4-Amino-2-styrylquinazolines - a new class of
antiprotozoal drugsAUTHOR(S): Moskalenko, N. Yu.; Yakhontov, L. N.; Zhikhareva, G.
P.; Pershin, G. N.; Peters, V. V.; Evstratova, M. I.;
Mastafanova, L. I.; Rabinovich, S. A.; Maksakovskaya,
E. V.; Kulikovskaya, I. M.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im.

Ordzhonikidze, Moscow, USSR

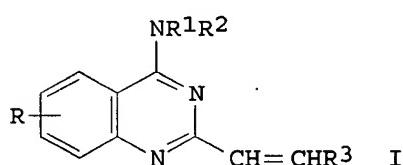
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1986), 20(4),
437-46

DOCUMENT TYPE: CODEN: KHFZAN; ISSN: 0023-1134

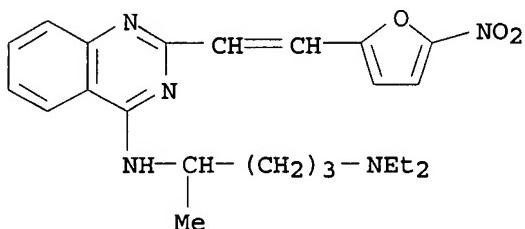
LANGUAGE: Journal

OTHER SOURCE(S): Russian

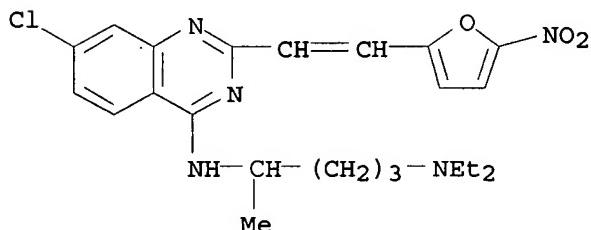
GI: OTHER SOURCE(S): CASREACT 106:32975



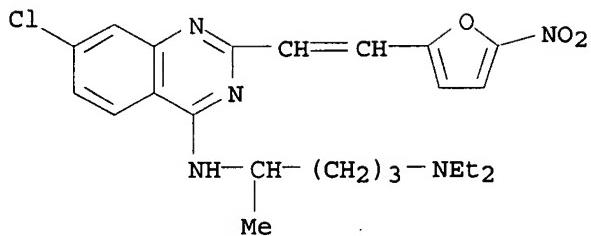
- AB 4-Amino-2-styrylquinazolines (I, R = H, 6-OMe, 7-Cl or 6-NO₂; NR₁R₂ = NHCHMe(CH₂)₃NET₂, Et₂N, piperidino or PhNH; and R₃ = 4-aminophenyl, 2-nitrophenyl, 4-nitrophenyl, 2-anisyl, 2-(2-nitrofuryl), or halophenyl, etc.,) were prepared by the reaction of the corresponding N-substituted-2-methylquinazolines with suitable aldehydes. Various pharmacol. activities of these compds., e.g., trypanosomicidal, amebicidal, protozoacidal, antimalarial, etc., were determined. The LD₅₀ for these compds. are tabulated. Against protozoal infections, 4-(8-diethylamino- α -methylbutylamino)-2-styrylquinazoline with a p-nitro group in the styrene ring showed the highest activity. Replacement of the nitro group by halogen atoms decreased the protozoacidal activity. The presence of the 4-8-diethylamino- α -methylbutylamino group in styrylquinazolines is necessary for exhibiting the antileishmaniasis activity. Other structure-activity correlations are discussed.
- IT 57942-39-9P 69258-64-6P 105997-20-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and protozoacidal activity of)
- RN 57942-39-9 ZCPLUS
- CN 1,4-Pentanediamine, N1,N1-diethyl-N4-[2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]- (9CI) (CA INDEX NAME)



- RN 69258-64-6 ZCPLUS
- CN 1,4-Pentanediamine, N4-[7-chloro-2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]-N1,N1-diethyl- (9CI) (CA INDEX NAME)



- RN 105997-20-4 ZCPLUS
- CN 1,4-Pentanediamine, N4-[7-chloro-2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]-N1,N1-diethyl-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

L4 ANSWER 22 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1980:514434 ZCPLUS

DOCUMENT NUMBER: 93:114434

TITLE: Synthesis and antiinflammatory activity of substituted
2-styryl-4-[δ -diethylamino- α -
methylbutylamino]-6-nitro- and 2-styryl-4-[δ -
diethylamino- α -methylbutylamino]-6-
aminoquinazolinesAUTHOR(S): Zhikhareva, G. P.; Mastafanova, L. I.; Evstratova, M.
I.; Shvarts, G. Ya.; Syubaev, R. D.; Mashkovskii, M.
D.; Yakhontov, L. N.CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1980), 14(2), 45-9
CODEN: KHFZAN; ISSN: 0023-1134DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

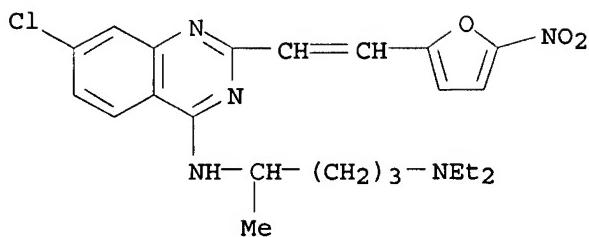
AB Treatment of 2-methyl-6-nitro-4-quiazolone with POCl₃ gave 51% quiazoline I (R = Cl) which was converted to 76% I (R = CHMe(CH₂)₃NET₂) (II) by reaction with the appropriate amine. Condensation of aldehydes with II gave III (R₁ = NO₂, R₂-6 = F; R₂ = R₄ = R₆ = Cl, R₃ = R₅ = H), which were reduced to give III (R₄ = NH₂). II (R₁ = NH₂, NO₂), IV (R₁ = R₃ = H, R₂ = R₄ = Cl; R₂ = R₃ = H, R₁ = R₄ = Cl; R₂ = R₄ = H, R₁ = Cl, R₃ = MeO; R₁ = R₃ = H, R₂ = NO₂, R₄ = Cl; R₁ = R₄ = H, R₂ = NO₂, R₃ = MeO) and 14 V (R₁, R₂, R₃, R₄, R₅ = Cl, MeO, Br, H, NO₂) were tested for their antiinflammatory, analgesic and antipyretic activity and most had LD >1000 mg/kg. Several of the compds. had biol. activity.

IT 69258-64-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, antipyretic, antiinflammatory, and analgesic activity of)

RN 69258-64-6 ZCPLUS

CN 1,4-Pentanediamine, N4-[7-chloro-2-[2-(5-nitro-2-furanyl)ethenyl]-4-
quinazolinyl]-N1,N1-diethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 23 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1979:121527 ZCPLUS

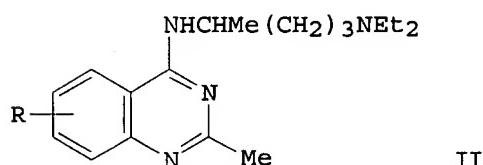
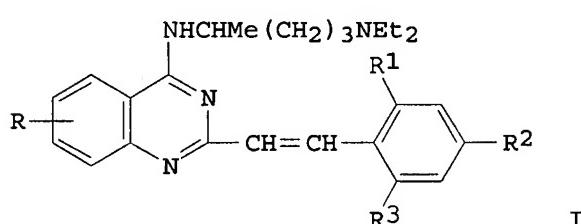
DOCUMENT NUMBER: 90:121527

TITLE: Synthesis and study of the antiviral activity of substituted 4-(δ -diethylamino- α -methylbutylamino)-2-styrylquinazolines

AUTHOR(S): Zhikhareva, G. P.; Mastafanova, L. I.; Bogdanova, N. S.; Peters, V. V.; Nikolaeva, I. S.; Pershin, G. N.; Yakhontov, L. N.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1978), 12(11), 44-8DOCUMENT TYPE: CODEN: KHFZAN; ISSN: 0023-1134
Journal

LANGUAGE: Russian

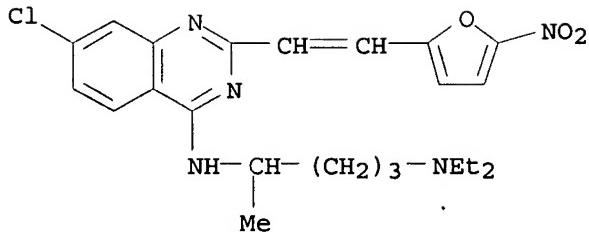
OTHER SOURCE(S): CASREACT 90:121527
GIAB The title compds. I ($R = H, 7\text{-Cl}, 6\text{-MeO}$, $R1 = Cl, Br, H$, $R2 = H, Br, Cl, NO_2$, $R3 = H, Cl$) and their hydrochlorides, useful as virucides, were obtained in 41-56% yields by condensation of II with substituted benzaldehydes.

IT 69258-64-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and virucidal activity of)

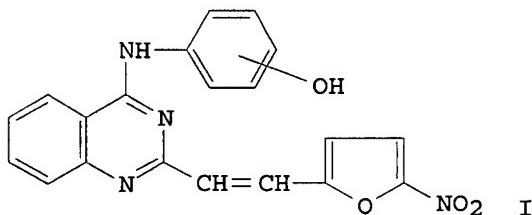
RN 69258-64-6 ZCPLUS

CN 1,4-Pentanediamine, N4-[7-chloro-2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]-N1,N1-diethyl- (9CI) (CA INDEX NAME)

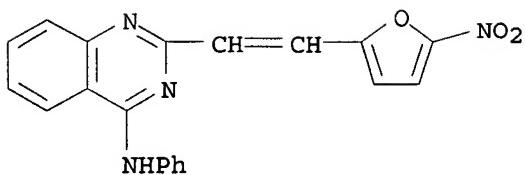


L4 ANSWER 24 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1977:16693 ZCPLUS
 DOCUMENT NUMBER: 86:16693
 TITLE: 2-[2-(5-Nitro-2-furyl)vinyl]-4-(hydroxyanilino)quinazolines
 INVENTOR(S): Horn, Herman; Greenbaum, Sheldon B.; Ely, Charles M.; Hacke, Walter; Olle, David A.
 PATENT ASSIGNEE(S): Diamond Shamrock Corp., USA
 SOURCE: U.S., 9 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 3970648 | A | 19760720 | US 1974-503854 | 19740906 |
| US 3973021 | A | 19760803 | US 1975-567499 | 19750414 |
| US 3974277 | A | 19760810 | US 1975-570645 | 19750423 |
| PRIORITY APPLN. INFO.: | | | US 1974-503854 | A3 19740906 |
| GI | | | | |



- AB The title compds. I, bactericides and growth promoters for chicks, and the bactericidal anilino analog were prepared from the 4-chloroquinazoline analog. Thus, 9.05 g the 4-chloro analog of I, prepared by chlorination of the condensation product of 5-nitro-2-furancarboxaldehyde and 2-methyl-4(3H)quinazolinone, and 8 g 4-H2NC6H4OH in DMF was heated 2 hr at 70-90° to give 6-5 g I (OH in 4-position).
- IT 60535-07-1P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and bactericidal activity of)
- RN 60535-07-1 ZCPLUS
- CN 4-Quinazolinamine, 2-[2-(5-nitro-2-furyl)ethenyl]-N-phenyl- (9CI) (CA INDEX NAME)



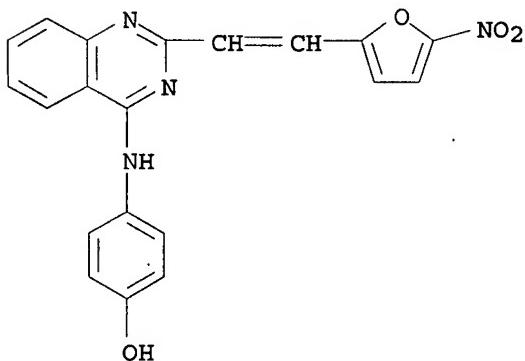
IT 60452-41-7 60452-42-8 60452-43-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation as bactericidal and animal growth substances)

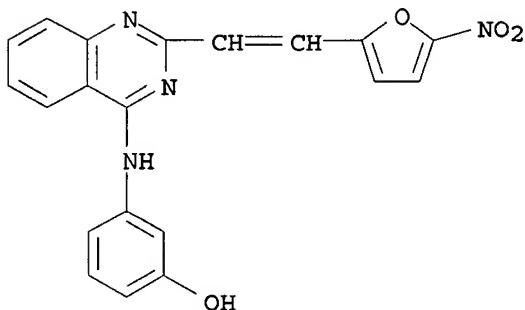
RN 60452-41-7 ZCPLUS

CN Phenol, 4-[(2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl)amino]- (9CI)
(CA INDEX NAME)



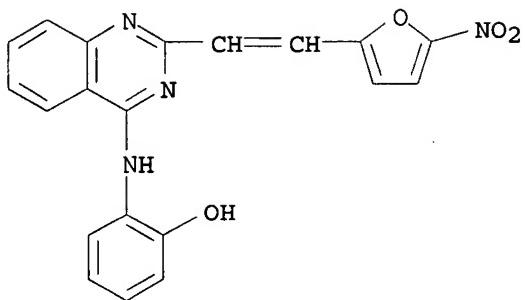
RN 60452-42-8 ZCPLUS

CN Phenol, 3-[(2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl)amino]- (9CI)
(CA INDEX NAME)

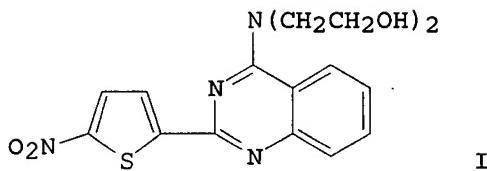


RN 60452-43-9 ZCPLUS

CN Phenol, 2-[(2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl)amino]- (9CI)
(CA INDEX NAME)



L4 ANSWER 25 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1976:572499 ZCPLUS
 DOCUMENT NUMBER: 85:172499
 TITLE: Comparative carcinogenicity of 5-nitrothiophenes and 5-nitrofurans in rats
 AUTHOR(S): Cohen, Samuel M.; Erturk, E.; Bryan, George T.
 CORPORATE SOURCE: Cent. Health Sci., Univ. Wisconsin, Madison, WI, USA
 SOURCE: Journal of the National Cancer Institute (1940-1978)
 (1976), 57(2), 277-82
 CODEN: JNCIAM; ISSN: 0027-8874
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The carcinogenicity of five 5-nitrothiophenes with heterocyclic substituents at the 2-position of the thiophene ring was investigated by feeding the chems. to Sprague-Dawley rats and comparing the type and incidence of lesions with those appearing after exposure to two 5-nitrofurans. Benign and malignant mammary tumors and intestinal tract sarcomas were the most frequent lesions induced by 5-nitrothiophenes. 4-Bis(2-hydroxyethyl)amino-2-(5-nitro-2-thienyl)quinazoline (I) [33372-39-3] caused a 100% incidence of mammary adenocarcinomas in 28 female rats at risk; it induced 3 benign and 5 malignant mammary tumors and 13 small intestine sarcomas in 20 male rats. A high incidence of similar lesions was observed in male and female rats fed the corresponding 5-nitrofuran analogue, 4-bis(2-hydroxyethyl)amino-2-(5-nitro-2-furyl)quinazoline [5055-20-9]. In marked contrast, 4 of 28 female rats receiving 4-bis(2-hydroxyethyl)amino-2-(2-thienyl)quinazoline [58139-47-2], which lacks the nitro group at the 5-position on the thiophene ring, had solitary benign mammary tumors. Addnl. 5-nitrothiophenes demonstrating significant oncogenic activity for female rats were 4-morpholino-2-(5-nitro-2-thienyl)quinazoline [58139-48-3], 4-(2-hydroxyethylamino)-2-(5-nitro-2-thienyl)quinazoline [33389-36-5], 4-(2,3-dihydroxypropylamino)-2-(5-nitro-2-thienyl)quinazoline [33372-40-6], and 1,2-dihydro-2-(5-nitro-2-thienyl)quinazolin-4(3H)-one [33389-33-2]. Another nitrofuran, 4,6-dimethyl-2-(5-nitro-2-furyl)-pyrimidine [59-35-8], provided the following types of neoplasms in 30 female rats at risk: squamous cell carcinomas of the forestomach (30),

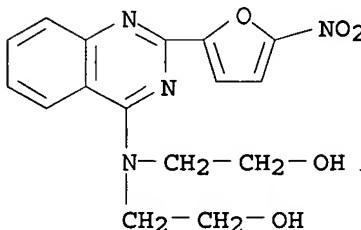
sarcomas of the intestine (21), adenocarcinomas of the mammary gland (12), and transitional cell carcinomas of the kidney (2).

IT 5055-20-9

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(carcinogenicity of)

RN 5055-20-9 ZCPLUS

CN Ethanol, 2,2'-[2-(5-nitro-2-furanyl)-4-quinazolinyl]imino]bis- (9CI) (CA
INDEX NAME)



L4 ANSWER 26 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:558452 ZCPLUS

DOCUMENT NUMBER: 85:158452

TITLE: 2-[2-(5-Nitro-2-furyl)vinyl]-4-(p-hydroxyanilino)quinazoline as a bactericide

INVENTOR(S): Horn, Herman; Greenbaum, Sheldon B.; Ely, Charles M.; Hacke, Walter; Olle, David A.

PATENT ASSIGNEE(S): Diamond Shamrock Corp., USA

SOURCE: U.S., 9 pp.
CODEN: USXXAM

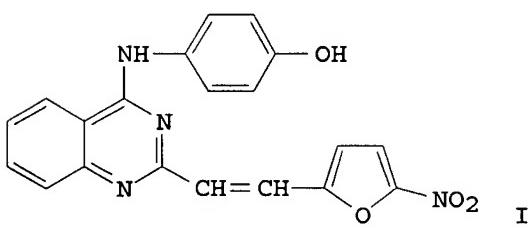
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------------|------|----------|-----------------|-------------|
| US 3973021 | A | 19760803 | US 1975-567499 | 19750414 |
| US 3970648 | A | 19760720 | US 1974-503854 | 19740906 |
| PRIORITY APPLN. INFO.: GI | | | US 1974-503854 | A3 19740906 |



AB 2-[2-(5-Nitro-2-furyl)vinyl]-4-(p-hydroxyanilino)quinazoline (I) [60452-41-7] and similar quinazolines are effective as bactericides and animal growth promoting agents. Thus, broiler chicks given I at 200 g/ton of feed gained 6.5% more weight than controls fed the basal ration plus bacitracin in 4-week expts.; bacitracin plus chlortetracycline at 4 and 200 g/ton, resp. gave only 5.5% better growth, as compared to controls.. Feed efficiency also was improved with addition of I by 7.2% as compared to 6.6% with chlortetracycline.

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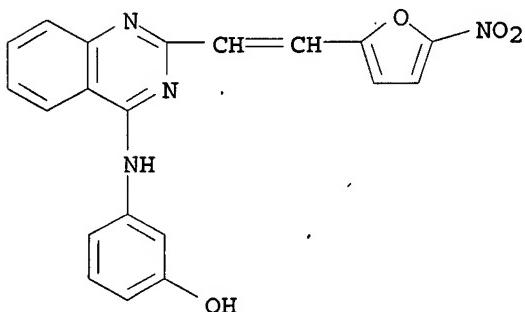
IT 60452-42-8P 60452-43-9P 60535-07-1P

RL: PREP (Preparation)

(preparation and feeding experiment on chicks with)

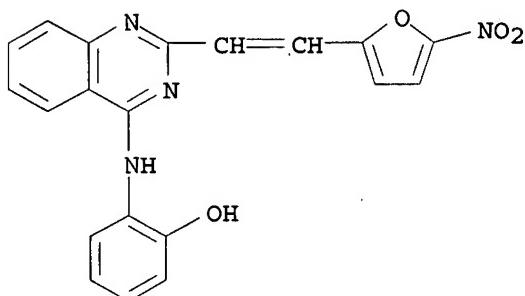
RN 60452-42-8 ZCPLUS

CN Phenol, 3-[[2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]amino]- (9CI)
(CA INDEX NAME)



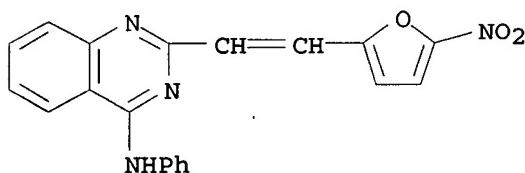
RN 60452-43-9 ZCPLUS

CN Phenol, 2-[[2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]amino]- (9CI)
(CA INDEX NAME)



RN 60535-07-1 ZCPLUS

CN 4-Quinazolinamine, 2-[2-(5-nitro-2-furanyl)ethenyl]-N-phenyl- (9CI) (CA INDEX NAME)



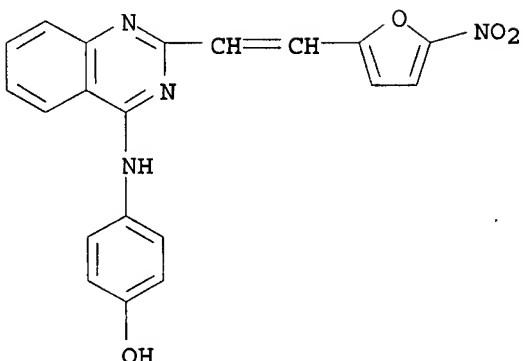
IT 60452-41-7P

RL: PREP (Preparation)

(preparation and feeding expts. with, on chicks and pigs)

RN 60452-41-7 ZCPLUS

CN Phenol, 4-[[2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]amino]- (9CI)
(CA INDEX NAME)



L4 ANSWER 27 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:541790 ZCPLUS

DOCUMENT NUMBER: 85:141790

TITLE: 2-[2-(5-Nitro-2-furyl)vinyl]-4-(anilino)quinazolines
as growth promotants and feed efficiency enhancing
agentsINVENTOR(S): Horn, Herman; Greenbaum, Sheldon B.; Ely, Charles M.;
Hacke, Walter; Olle, David A.

PATENT ASSIGNEE(S): Diamond Shamrock Corp., USA

SOURCE: U.S., 10 pp.
CODEN: USXXAM

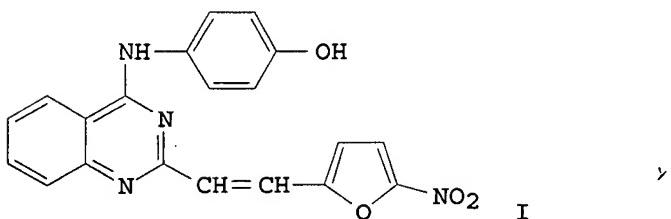
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------------|-----------------|-------------|
| US 3974277 | A | 19760810 | US 1975-570645 | 19750423 |
| US 3970648 | A | 19760720 | US 1974-503854 | 19740906 |
| PRIORITY APPLN. INFO.: | | US 1974-503854 | | A3 19740906 |
| GI | | | | |



AB The title compds. and derivs. are prepared and found useful as bactericides and animal growth promotants. For example, 2-[2-(5-nitro-2-furyl)vinyl]-4-(p-hydroxyanilino)quinazoline (I) [60452-41-7], prepared by reacting 2-[2-(5-nitro-2-furyl)vinyl]-4-chloroquinazoline [36952-05-3] with p-aminophenol [123-30-8], when added at 200 g/ton to a com.-type chick starter ration containing 4 g bacitracin/ton, increased 4-week growth and feed efficiency to 106 and 107%, resp., of that obtained from the com. diet + bacitracin alone.

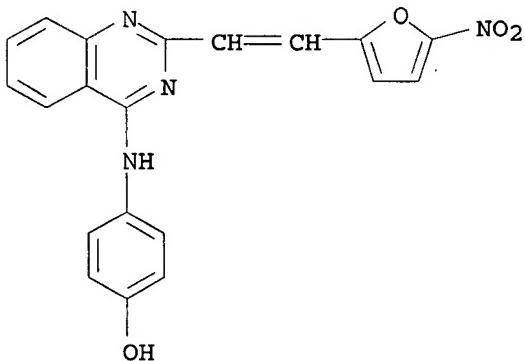
IT 60452-41-7P

RL: PREP (Preparation)

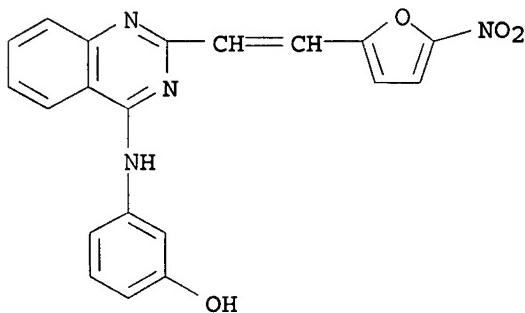
(preparation and bactericidal and animal growth promotant properties of)

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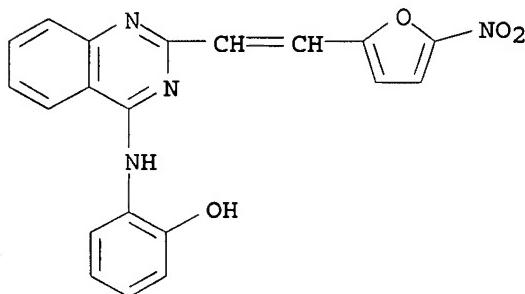
RN 60452-41-7 ZCPLUS
CN Phenol, 4-[[2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]amino]- (9CI)
(CA INDEX NAME)



IT 60452-42-8P 60452-43-9P
RL: PREP (Preparation)
(preparation and bactericidal and animal growth stimulant properties of)
RN 60452-42-8 ZCPLUS
CN Phenol, 3-[[2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]amino]- (9CI)
(CA INDEX NAME)

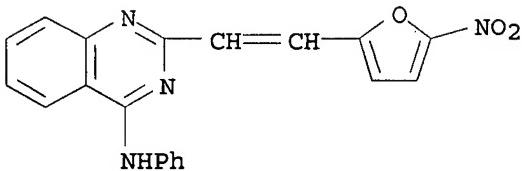


RN 60452-43-9 ZCPLUS
CN Phenol, 2-[[2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]amino]- (9CI)
(CA INDEX NAME)



IT 60535-07-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and bactericidal properties of)
RN 60535-07-1 ZCPLUS

CN 4-Quinazolinamine, 2-[2-(5-nitro-2-furanyl)ethenyl]-N-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 28 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:43974 ZCPLUS

DOCUMENT NUMBER: 84:43974

TITLE: Synthesis and study of the biological activity of substituted 4-amino-2-styrylquinazolines

AUTHOR(S): Yakhontov, L. N.; Zhikhareva, G. P.; Pronina, E. V.; Pershin, G. N.; Liberman, S. S.; Padeiskaya, E. N.; Zykova, T. N.; Gus'kova, T. A.; Berlyand, E. A.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1975), 9(11), 12-18

DOCUMENT TYPE: CODEN: KHFZAN; ISSN: 0023-1134

LANGUAGE: Journal

OTHER SOURCE(S): Russian

GI For diagram(s), see printed CA Issue.

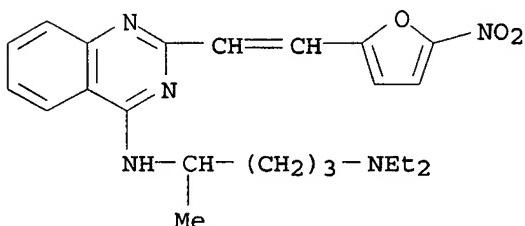
AB Aminostyrylquinazolines [I, R = Cl, H, NR₁R₂ = Et₂N, PhNH, PhCH₂NH, Et₂N(CH₂)₃CHMeNH, piperidino, R₃ = o-, p-Cl, p-O₂N] were obtained in 28-66% yields in 5 steps from anthranilic acid derivs. by cyclocondensation with Ac₂O, treatment with NH₃ to give II, chlorination with POCl₃, amination with R₁R₂NH, and condensation with the corresponding aromatic aldehyde. I were effective bactericides against Mycobacterium tuberculosis at 0.25-0.5 µg/ml.

IT 57942-39-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 57942-39-9 ZCPLUS

CN 1,4-Pentanediamine, N₁,N₁-diethyl-N₄-[2-[2-(5-nitro-2-furanyl)ethenyl]-4-quinazolinyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 29 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1975:479282 ZCPLUS

DOCUMENT NUMBER: 83:79282

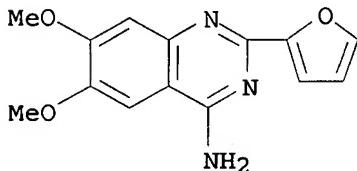
TITLE: Bactericidal and antihypertensive 4-aminoquinazoline compounds

INVENTOR(S): Nauta, Wijbe T.

PATENT ASSIGNEE(S): N. V. Koninklijke Pharmaceutische Fabrieken Voorheen

SOURCE: Brocades-Stheeman & Pharmacia, Neth.
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|------------|
| GB 1390015 | A | 19750409 | GB 1974-47849 | 19720505 |
| | | | GB 1974-47849 | A 19720505 |
| PRIORITY APPLN. INFO.: | | | | |
| GI | For diagram(s), see printed CA Issue. | | | |
| AB | Ten title compds. I (R = pyrrolidyl, 2-, 3-, and 4-pyridyl, 2-furyl, 1-methyl-2-pyrrolyl; R1 = H, Cl, MeO; R2 = H, MeO) were prepared from 2-aminobenzonitriles by treatment with heterocyclic nitriles. Thus, I (R = pyrrolidyl, R1 = R2 = H) was prepared from 2-H2NC6H4CN in Et2O by refluxing with 1-pyrrolidinonitrile 4 hr under N in the presence of PhBr-Li followed by treatment with H2O. I showed bactericidal activity (no data) towards Mycoplasma gallisepticum and Pasteurella multocida. The antihypertensive activities of I were assessed in rats (no data). | | | |
| IT | 56503-36-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(bactericide and antihypertensive, preparation of) | | | |
| RN | 56503-36-7 ZCPLUS | | | |
| CN | 4-Quinazolinamine, 2-(2-furanyl)-6,7-dimethoxy-, monohydrochloride (9CI)
(CA INDEX NAME) | | | |



● HCl

L4 ANSWER 30 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1973:72180 ZCPLUS
 DOCUMENT NUMBER: 78:72180
 TITLE: Pyrimidine derivatives
 PATENT ASSIGNEE(S): N. V. Koninklijke Pharmaceutische Fabrieken Voorheen Brocades-Stheeman & Pharmacia
 SOURCE: Neth. Appl., 19 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Dutch
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| NL 7206067 | A | 19721109 | NL 1972-6067 | 19720505 |
| JP 56001315 | B | 19810113 | JP 1972-44512 | 19720504 |
| NO 139270 | C | 19790131 | NO 1972-1600 | 19720505 |
| NO 139270 | B | 19781023 | | |
| SE 406197 | C | 19790510 | SE 1972-5960 | 19720505 |

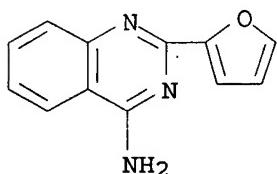
SE 406197

B 19790129

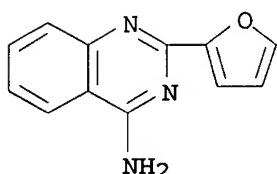
GB 1971-13802

A 19710507

PRIORITY APPLN. INFO.: GI For diagram(s), see printed CA Issue.
 AB Aminoquinazolines (I, R = NMe₂, NEt₂, pyrrolidino, 2-furyl, 2-pyridyl, 1-methyl-2-pyrrolyl, 4-(2-furoyl)-1-piperazinyl; R₁ = R₂ = H, OMe; R₁ = Cl, R₂ = H) were prepared by treating the corresponding o-aminobenzonitrile with RCN and PhLi. Thus, reaction of o-H₂NC₆H₄CN with Et₂N₂CN and PhLi gave I (R = NEt₂, R₁ = R₂ = H).
 IT 40172-85-8P 40172-86-9P 40173-00-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 40172-85-8 ZCPLUS
 CN 4-Quinazolinamine, 2-(2-furanyl)- (9CI) (CA INDEX NAME)

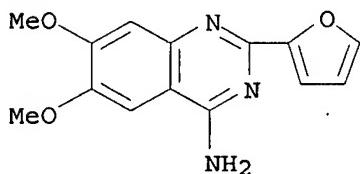


RN 40172-86-9 ZCPLUS
 CN 4-Quinazolinamine, 2-(2-furanyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 40173-00-0 ZCPLUS
 CN 4-Quinazolinamine, 2-(2-furanyl)-6,7-dimethoxy-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

TITLE: 4-Amino-2-[2-(5-nitro-2-furyl)vinyl]quinazolines
 INVENTOR(S): Breuer, Hermann
 PATENT ASSIGNEE(S): Chemische Fabrik von Heyden A.-G.
 SOURCE: Ger. Offen., 12 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|------------|
| DE 2140280 | A | 19720217 | DE 1971-2140280 | 19710811 |
| FR 2102221 | A5 | 19720407 | FR 1971-29610 | 19710812 |
| FR 2102221 | B1 | 19750207 | | |
| CH 529781 | A | 19721031 | CH 1971-529781 | 19710812 |
| | | | US 1970-63327 | A 19700812 |

PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

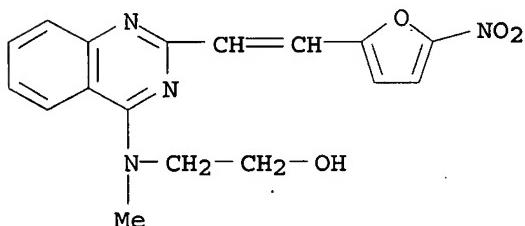
AB Six title compds. [I, R₁ = H, R = morpholino (II), N(CH₂CH₂OH)₂ NETCH₂CH₂OH or NMeCH₂CH₂OH; and R = morpholino, R₁ = Cl or NO₂], useful as antimicrobial agents in animals, were prepared by reaction of I (R = Cl) with amines. Thus I (R = Cl, R₁ = H), prepared from 2-methyl-4(3H)-quinazolinone and 5-nitro-2-furaldehyde via 2-[2-(5-nitro-2-furyl)vinyl]-4(3H)-quinazolinone followed by reaction with POCl₃ in PhNMe₂, was treated with morpholine in PhMe for 0.5 hr at 70-80° to give II.

IT 36951-95-8P 36951-96-9P 36952-03-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

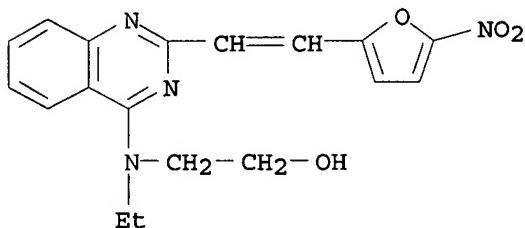
RN 36951-95-8 ZCPLUS

CN Ethanol, 2-[methyl[2-[2-(5-nitro-2-furyl)ethenyl]-4-quinazolinyl]amino] - (9CI) (CA INDEX NAME)



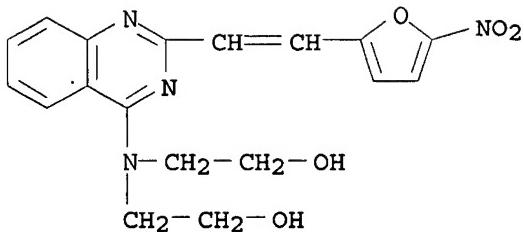
RN 36951-96-9 ZCPLUS

CN Ethanol, 2-[ethyl[2-[2-(5-nitro-2-furyl)ethenyl]-4-quinazolinyl]amino] - (9CI) (CA INDEX NAME)



RN 36952-03-1 ZCPLUS

CN Ethanol, 2,2'-[[2-[2-(5-nitro-2-furyl)ethenyl]-4-quinazolinyl]imino]bis- (9CI) (CA INDEX NAME)



L4 ANSWER 32 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1970:97625 ZCPLUS

DOCUMENT NUMBER: 72:97625

TITLE: Determination of untreated whole milk effects on in vitro antibacterial activity

AUTHOR(S): Van Natta, J. P.; Lo, P. W.; Chang, Timothy Scott

CORPORATE SOURCE: Res. Develop. Dep., Norwich Pharmacal Co., Norwich, NY, USA

SOURCE: Applied Microbiology (1970), 19(2), 220-3

CODEN: APMBAY; ISSN: 0003-6919

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effect of fresh whole milk without pasteurization or other pretreatment on in vitro antibacterial activity of selected compds. was determined in broth dilution. The milk was collected by hand directly from dairy

goats, or by syringe or cannula from bovine quarters showing low bacterial counts. Antibacterial activity was determined in 50% (v/v) milk-broth medium against sensitive mastitisetiologic strains of *Streptococcus agalactiae* and *Staphylococcus aureus*. The indicator sale 2,3,5-triphenyltetrazolium chloride was incorporated in the milk-broth medium to determine inoculum growth. Contaminant interference was circumvented through early as well as late readings and comparisons with uninoculated control tubes, with and without the test compds. Application of the method with more than 75 compds., including nitrofurans, antibiotics, and other chems. uncovered marked degrees of milk interference. The method warrants routine use among preliminary screens to relate in vitro with in vivo observations of antimicrobial activity. Similar procedures may be used with serum, skim milk, or mastitis-milk media for separating effects due to protein, lipid, or other elements in product evaluation.

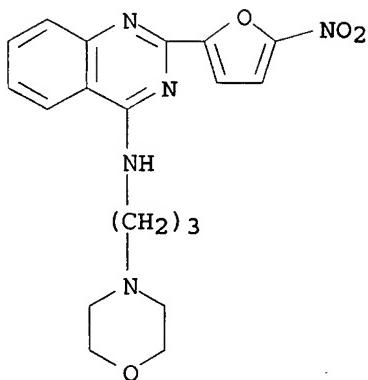
IT 5489-93-0 27465-08-3 27465-09-4

27465-10-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antibiotic activity of, milk effect on)

RN 5489-93-0 ZCPLUS

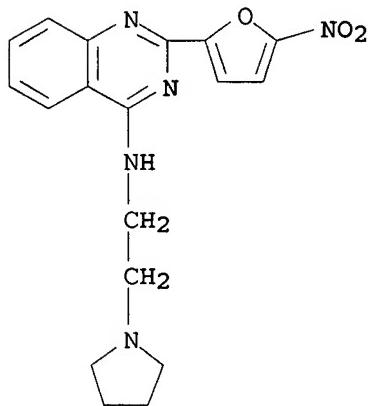
CN 4-Quinazolinamine, N-[3-(4-morpholinyl)propyl]-2-(5-nitro-2-furanyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 27465-08-3 ZCPLUS

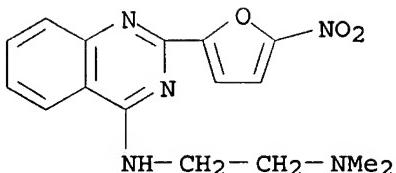
CN Quinazoline, 2-(5-nitro-2-furyl)-4-[(2-(1-pyrrolidinyl)ethyl)amino]-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



●x HCl

RN 27465-09-4 ZCPLUS

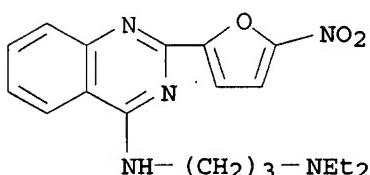
CN Quinazoline, 4-[(2-(dimethylamino)ethyl)amino]-2-(5-nitro-2-furyl)-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



●x HCl

RN 27465-10-7 ZCPLUS

CN Quinazoline, 4-[3-(diethylamino)propyl]amino]-2-(5-nitro-2-furyl)-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



●x HCl

L4 ANSWER 33 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1970:31830 ZCPLUS

DOCUMENT NUMBER: 72:31830

TITLE: Bactericidal 4-(o-, m-, and p-hydroxyanilino)-2-(5-nitro-2-furyl)quinazolines

PATENT ASSIGNEE(S): Norwich Pharmacal Co.

SOURCE: Brit., 3 pp.
CODEN: BRXXAA

DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|-------|----------|-----------------|----------|
| GB 1168430 | ----- | 19691022 | GB 1969-4748 | 19690128 |
| DE 1909522 | ----- | | DE | |
| FR 2005591 | ----- | | FR | |
| US 3542784 | ----- | 19701124 | US | 19680405 |
| ZA 6900771 | ----- | 19690000 | ZA | |
| PRIORITY APPLN. INFO.: | | | US | 19680405 |

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) in which the OH may be in the 2-, 3-, or 4-position show high in vitro antibacterial activity. A mixture of 35 g II and 28.5 g o-HOC6H4NH2 in 500 ml Me2NCHO was heated on the steam-bath 2 hr to give 35 g I (2-OH) (III), m. 275° (decomposition). Similarly were prepared I (3-OH) (IV), m. 284° (decomposition) and I (4-OH), m. 286-8° (decomposition). I were particularly effective in vitro against animal pathogens.

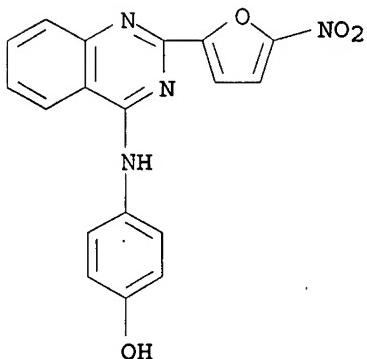
IT 24912-15-0P 24912-16-1P 24912-17-2P

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RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

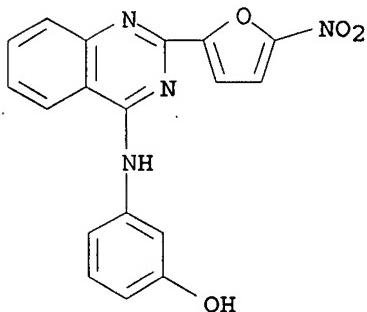
RN 24912-15-0 ZCPLUS

CN Phenol, p-[(2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- (8CI) (CA INDEX
NAME)



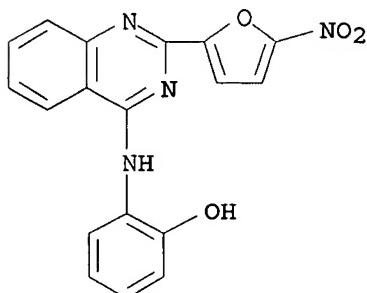
RN 24912-16-1 ZCPLUS

CN Phenol, m-[(2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- (8CI) (CA INDEX
NAME)



RN 24912-17-2 ZCPLUS

CN Phenol, o-[(2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- (8CI) (CA INDEX
NAME)



L4 ANSWER 34 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:490697 ZCPLUS
DOCUMENT NUMBER: 65:90697
ORIGINAL REFERENCE NO.: 65:16981h,16982a-f

TITLE: 4-Substituted 2-(5-nitro-2-furyl)quinazolines
 INVENTOR(S): Burch, H. A.
 PATENT ASSIGNEE(S): Norwich Pharmacal Co.
 SOURCE: 17 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|----------|
| BE 672504 | | 19660316 | BE 1967-2504 | 19651118 |
| PRIORITY APPLN. INFO.: | | | US | 19641214 |

GI For diagram(s), see printed CA Issue.

AB The title products with general formula (I), useful as antibacterials, are prepared CaCO_3 (5 g.) is added to a solution of 6.8 g. o-aminobenzamide in 30 cc. HCONMe_2 . A solution of 8.75 g. 5-nitrofuroyl chloride in 20 cc. HCONMe_2 is added with stirring. The mixture is heated for 1 hr., filtered, and cooled. The precipitate is filtered, and crystallized from HCONMe_2 to give

3.9 g.

2-(5-nitro-2-furyl)-4(3H)-quinazolinone (II). II (198 g.) is added slowly with stirring to a solution of 159 g. PCl_5 in 790 cc. POCl_3 . The mixture is refluxed for 1 hr., cooled, diluted with 3000 cc. petroleum ether, and cooled again. The precipitate is filtered off and purified by extraction with toluene

in a Soxhlet apparatus The toluene solution is cooled, and the precipitate filtered to

give 106 g. 4-chloro-2-(5-nitro-2-furyl)quinazoline (III), m.

196.5-8.5°. A solution of 30 g. III and 26.5 g. $\text{HOCHMeCH}_2\text{NH}(\text{CH}_2)_2\text{OH}$ in 750 cc. HCONMe_2 is heated on a steam bath for 1 hr., diluted with water, and cooled. The precipitate is filtered off to give 18 g. 4-[2-hydroxyethyl (2-hydroxy-1-propyl)amino]-2-(5-nitro-2-furyl)quinazoline, m. 165-6° (all m.ps. are corrected) (iso-PrOH). A solution of 40 g. III and 40 g. $(\text{HOCHMeCH}_2)_2\text{NH}$ in 500 cc. HCONMe_2 is heated on a steam bath for 2 hrs., diluted with water, and cooled to give 39 g. 4-bis(2-hydroxy-1-propyl)amino-2-(5-nitro-2-furyl)quinazoline, m. 169-70°. In the same way, 40 g.

III, 36 g. N-butylethanolamine, and 500 cc. HCONMe_2 give 39 g.

4-butyl(2-hydroxyethyl)amino-2-(5-nitro-2-furyl)quinazoline, m.

120-1°; 30.2 g. III, 26.3 g. diethanolamine, and 300 cc. HCONMe_2 give 22 g. 4-bis(2-hydroxyethyl)amino-2-(5-nitro-2-furyl)quinazoline, m.

167-8°; 35 g. III, 23.1 g. 3-methoxypropylamine, and 500 cc.

HCONMe_2 give 33 g. 4-(3-methoxypropylamino)-2-(5-nitro-2-

furyl)quinazoline, m.p. 143-5°; 35 g. III, 42 g.

diethoxyethylamine, and 1000 cc. HCONMe_2 give 40 g. 4-bis(2-

ethoxyethyl)amino-2-(5-nitro-2-furyl)quinazoline, m. 60-1°; 30.2 g.

III, 15 g. 2-ethanolamine, and 800 cc. HCONMe_2 give 31 g.

4-(2-hydroxyethyl)amino-2-(5-nitro-2-furyl)quinazoline, m. 221-3°;

and 35 g. III, 25 g. N-isopropylethanolamine, and 500 cc. HCONMe_2 give 21 g.

4-[(2-hydroxyethyl)isopropylamino]-2-(5-nitro-2-furyl)quinazoline, m.

157-9°. A mixture of 50 g. III, 34 g. N-methylethanolamine, and 1000 cc. benzene is refluxed for 1 hr., and cooled. The precipitate is filtered,

suspended in cool water, and alkalized with aqueous NaOH to give 40 g.

4-[(2-hydroxyethyl) methylamino]-2-(5-nitro-2-furyl)-quinazoline, m.

151-2° (HCONMe_2 -water). A mixture of 40 g. III, 22.5 g.

2-methoxyethylamine, and 1000 cc. benzene is refluxed for 1 hr., cooled, and diluted with petroleum ether to give 26 g. 4-(2-methoxyethyl)amino-2-(5-nitro-2-furyl)quinazoline, m.p. 160-2° (MeOH). A mixture of 30.2 g.

III, 36 g. 3-aminopropyl-4-morpholine, and 750 cc. benzene is refluxed for 1.5 hrs., cooled, and diluted with petroleum ether. The precipitate is filtered,

suspended in water, and alkalized with aqueous NaOH. The precipitate is filtered to

give 42 g. 4-[3-(4-morpholino)propyl]amino-2-(5-nitro-2-furyl)quinazoline

(IV), m. 170.0-1.5°. A solution of 40 g. IV in 500 cc. anhydrous AcOH is saturated with dry HCl while cooling, and diluted with ether to give 30 g. IV.2HCl, m. 211-13°. A solution of 35 g. III, and 19.5 g. 3-amino-1-propanol in 500 cc. HCONMe₂ is heated on a steam bath for 1 hr., diluted with water to give 22 g. 4-(3-hydroxy-1-propylamino)-2-(5-nitro-2-furyl)quinazoline, m.p. 180-3° (MeCN). A mixture of 40 g. III, 28.5 g. 80% 2-hydroxyethylhydrazine, and 500 cc. HCONMe₂ is left at room temperature for 15 min. and heated at 40°, and then at 60°. The solution is diluted with water to give 35.5 g. 4-[1-(2-hydroxyethyl)hydrazino]-2-(5-nitro-2-furyl)quinazoline, m.p. 190-1° (MeNO₂).

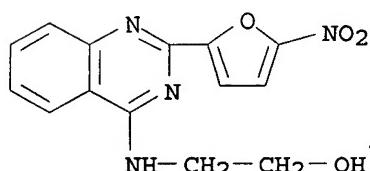
IT 5019-69-2P, Ethanol, 2-[(2-(5-nitro-2-furyl)-4-quinazolinyl]amino] - 5019-74-9P, 2-Propanol, 1,1'-[[2-(5-nitro-2-furyl)-4-quinazolinyl]imino]di- 5019-79-4P, Ethanol, 2-[1-[2-(5-nitro-2-furyl)-4-quinazolinyl]hydrazino] - 5055-18-5P, Ethanol, 2-[isopropyl[2-(5-nitro-2-furyl)-4-quinazolinyl]amino] - 5055-19-6P, Ethanol, 2-[butyl[2-(5-nitro-2-furyl)-4-quinazolinyl]amino] - 5055-20-9P, Ethanol, 2,2'--[[2-(5-nitro-2-furyl)-4-quinazolinyl]imino]di- 5055-21-0P, 2-Propanol, 1-[(2-hydroxyethyl)[2-(5-nitro-2-furyl)-4-quinazolinyl]amino] - 5055-30-1P, Quinazoline, 4-[(2-methoxyethyl)amino]-2-(5-nitro-2-furyl)- 5055-31-2P, Quinazoline, 4-[(3-methoxypropyl)amino]-2-(5-nitro-2-furyl)- 5055-33-4P, Quinazoline, 4-[bis(2-ethoxyethyl)amino]-2-(5-nitro-2-furyl)- 5085-66-5P, 1-Propanol, 3-[[2-(5-nitro-2-furyl)-4-quinazolinyl]amino] - 5094-03-1P, Ethanol, 2-[methyl[2-(5-nitro-2-furyl)-4-quinazolinyl]amino] - 5489-93-0P, Quinazoline, 4-[(3-morpholinopropyl)amino]-2-(5-nitro-2-furyl)-, dihydrochloride 10460-86-3P, Quinazoline, 4-[(3-morpholinopropyl)amino]-2-(5-nitro-2-furyl)-

RL: PREP (Preparation)

(preparation of)

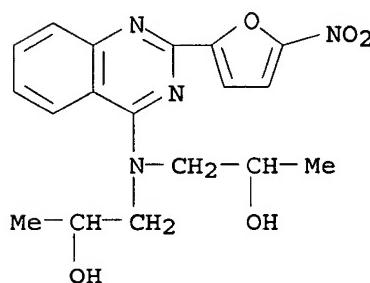
RN 5019-69-2 ZCPLUS

CN Ethanol, 2-[(2-(5-nitro-2-furanyl)-4-quinazolinyl]amino] - (9CI) (CA INDEX NAME)



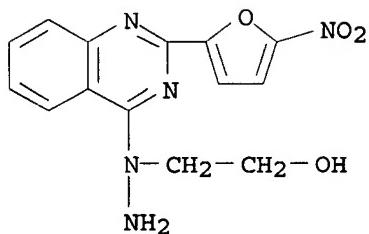
RN 5019-74-9 ZCPLUS

CN 2-Propanol, 1,1'-[[2-(5-nitro-2-furanyl)-4-quinazolinyl]imino]bis- (9CI) (CA INDEX NAME)



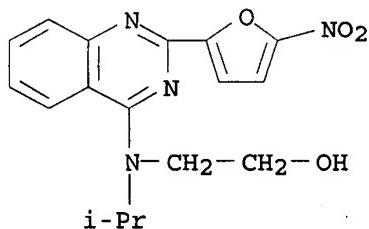
RN 5019-79-4 ZCPLUS

CN Ethanol, 2-[1-[2-(5-nitro-2-furanyl)-4-quinazolinyl]hydrazino] - (9CI) (CA INDEX NAME)



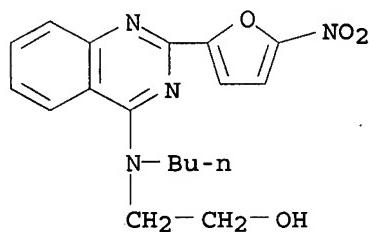
RN 5055-18-5 ZCPLUS

CN Ethanol, 2-[(1-methylethyl)[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



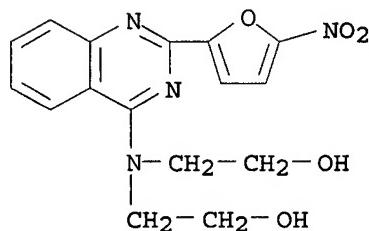
RN 5055-19-6 ZCPLUS

CN Ethanol, 2-[butyl[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



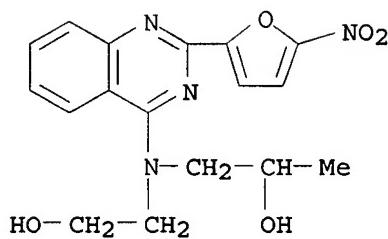
RN 5055-20-9 ZCPLUS

CN Ethanol, 2,2'-{[2-(5-nitro-2-furanyl)-4-quinazolinyl]imino}bis- (9CI) (CA INDEX NAME)



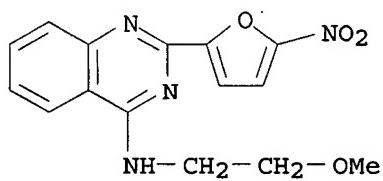
RN 5055-21-0 ZCPLUS

CN 2-Propanol, 1-[(2-hydroxyethyl)[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



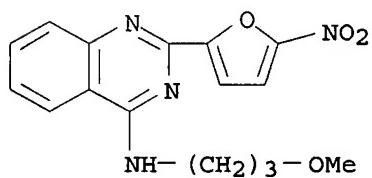
RN 5055-30-1 ZCPLUS

CN 4-Quinazolinamine, N-(2-methoxyethyl)-2-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)



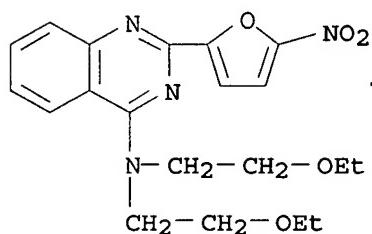
RN 5055-31-2 ZCPLUS

CN 4-Quinazolinamine, N-(3-methoxypropyl)-2-(5-(nitro-2-furanyl)- (9CI) (CA INDEX NAME)



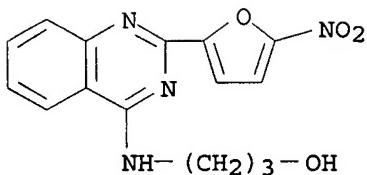
RN 5055-33-4 ZCPLUS

CN 4-Quinazolinamine, N,N-bis(2-ethoxyethyl)-2-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)

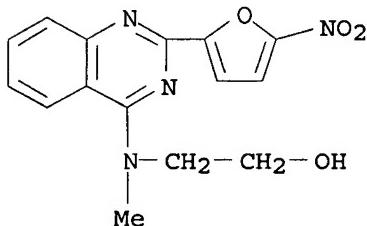


RN 5085-66-5 ZCPLUS

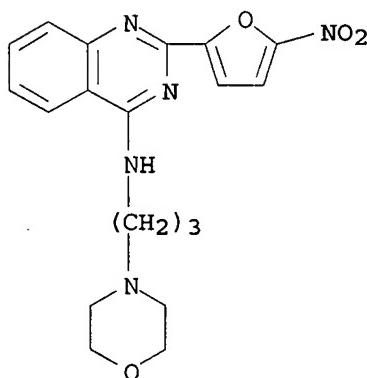
CN 1-Propanol, 3-[(2-(5-nitro-2-furanyl)-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)



RN 5094-03-1 ZCPLUS
CN Ethanol, 2-[methyl[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

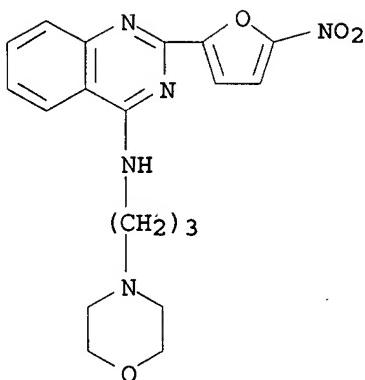


RN 5489-93-0 ZCPLUS
CN 4-Quinazolinamine, N-[3-(4-morpholinyl)propyl]-2-(5-nitro-2-furanyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 10460-86-3 ZCPLUS
CN Quinazoline, 4-[(3-morpholinopropyl)amino]-2-(5-nitro-2-furyl)- (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 35 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:403982 ZCPLUS

DOCUMENT NUMBER: 65:3982

ORIGINAL REFERENCE NO.: 65:710h, 711a-d

TITLE: Benzodiazines. VI. Synthesis of 2-substituted-4-hydrazinoquinazolines, 5-substituted [3,4-c]-s-triazolo-, and [1,5-c]tetrazoloquinazolines

AUTHOR(S): Postovskii, I. Ya.; Vereschagina, N. N.; Mertsalov, S. L.

CORPORATE SOURCE: S. M. Kirov Ural Polytech. Inst., Sverdlovsk

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1966), (1), 130-5

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB cf. CA 63, 13256g. 2-R-substituted quinazol-4-ones (I), -4-chloroquinazolines (II), and -4-hydrazinoquinazolines (III) were prepared. Treatment of II with CS(NH₂)₂ gave the corresponding isothiuronium salts, which on treatment with NaOH gave 2-R-substituted-quinazoline-4-thiones (IV). III with HNO₂ gave 5-R-substituted[1,5-c]tetrazoloquinazolines (V), with CH(OEt)₃ gave 5-R-substituted[3,4-c]-s-triazoloquinazolines (VI). V treated with HCl gave I (a, R = Me) (b, R = Ph) (c, R = α-furyl) (d, R = γ-pyridyl). Thus, 12.5 g. thioisonicotinamide and 12.5 g. anthranilic acid was heated at 150-60° 1 hr. to give 7.5 g. Id, m. 250° (dioxane). IIa-c were prepared according to Scarborough et al. (CA 57, 7263h). IIa m. 86-8° (heptane); IIb m. 124-6° (heptane); IIc m. 122-4° (heptane). A mixture of 7.5 g. Id, 60 cc. POCl₃, and 10 g. PCl₅ was boiled 4 hrs., POCl₃ distilled, the mixture poured onto ice, neutralized with NH₃, and filtered, the precipitate washed with H₂O

and

dried, the residue extracted with boiling C₆H₆, and the extract filtered and evaporated gave 6.5 g., IIId, m. 164-6° (heptane). II (0.02 mole) in C₆H₆ was stirred and cooled, 5-fold excess NH₂NH₂.H₂O in C₆H₆ added, and the mixture stirred 2 hrs. gave III. II (0.01 mole), 0.01 mole CS(NH₂)₂, and 50 cc. EtOH boiled 1 hr. and evaporated; the residue dissolved in NaOH, the mixture filtered, and the filtrate acidified with AcOH gave IV. The following III and IV were prepared (R, III m.p., III % yield, IV m.p., and IV % yield given): Me, 180-2° (CHCl₃), 80, 217-18° (EtOH), -; Ph, 214-15° (CHCl₃), 81, 216-18° (EtOH), 63; α-furyl, 249-50° (dioxane), 76, 219-20° (dioxane), 85; γ-pyridyl, 200-2° (CHCl₃), 97, -, -. Treatment of IIa with NH₂NH₂.H₂O in EtOH gave 50% N,N'-bis(2-methylquinazolyl)-4-hydrazine (VII), m. 280° (isoPrOH). III (0.002 mole) boiled 1 hr. with 5-fold excess CH(OEt)₃ gave VI. NaNO₂ (0.002 mole) was added to 0.002

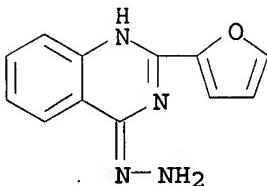
mole III in 2N HCl at 3-5° and the mixture stirred 1 hr. to give V. V were also prepared by treating II with NaN₃ in EtOH. The following VI and V were prepared (R, VI m.p., VI % yield, V m.p., and V % yield given): Me, >280°, 50, 163-5°, 60; Ph, 204-6°, 97, 162-3°, 70; α-furyl, 260-2°, 98, 194-6°, 73; γ-pyridyl, 206-7°, 80, 200-2°, 80. Boiling IV with 15-fold excess NH₂NH₂·H₂O in EtOH until no more H₂S evolved (8-10 hrs.) gave III. Treatment of V with HCl (1:1) 3 hrs. gave I. The compds. with R = Me differ considerably from the others, both in color and in stability of the intermediate reaction products.

IT 6505-41-5P, Quinazoline, 2-(2-furyl)-4-hydrazino-

RL: PREP (Preparation)
(preparation of)

RN 6505-41-5 ZCPLUS

CN Quinazoline, 2-(2-furyl)-4-hydrazino- (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 36 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:104206 ZCPLUS

DOCUMENT NUMBER: 64:104206

ORIGINAL REFERENCE NO.: 64:19608c-d

TITLE: Nitrofuryl heterocycles. IV. 4-Amino-2-(5-nitro-2-furyl)quinazoline derivatives

AUTHOR(S): Burch, Homer A.

CORPORATE SOURCE: Chem. Div., Norwich Pharmacal Co., Norwich, NY

SOURCE: Journal of Medicinal Chemistry (1966), 9(3), 408-10

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

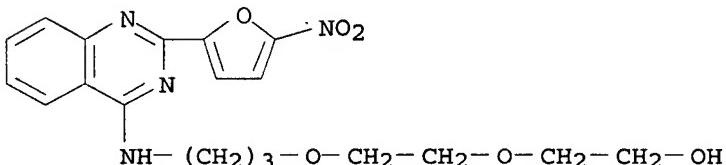
OTHER SOURCE(S): CASREACT 64:104206

AB cf. CA 64, 19596c. Thirty-five 4-(substituted amino)-2-(5-nitro-2-furyl)quinazolines were prepared and found to possess broad *in vitro* antibacterial activity against a variety of organisms. Several compds. were also active *in vivo* against *Staphylococcus aureus* infections. The most active compound contained the 4-bis(2-hydroxyethyl)amino group. A new mol. grouping responsible for enhancing the antibacterial activity of nitrofurans is postulated.

IT 5019-75-0, Ethanol, 2-[2-[3-[[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]propoxy]ethoxy]-
(others at q)

RN 5019-75-0 ZCPLUS

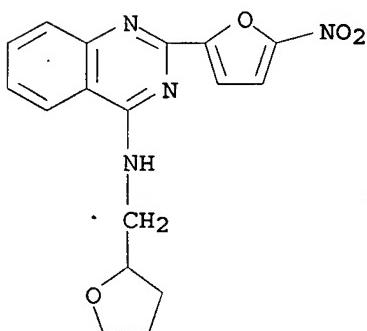
CN Ethanol, 2-[2-[3-[[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]propoxy]ethoxy]- (9CI) (CA INDEX NAME)



IT 5019-67-0P, Quinazoline, 2-(5-nitro-2-furyl)-4-[(tetrahydrofurfuryl)amino]- 5019-68-1P, Quinazoline, 4-(furfurylmethylamino)-2-(5-nitro-2-furyl)- 5019-69-2P, Ethanol, 2-[[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5019-70-5P, 2-Propanol, 1-[[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5019-71-6P, 1-Propanol, 2-methyl-2-[[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5019-72-7P, 1,2-Propanediol, 3-[[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5019-73-8P, Ethanol, 2-[benzyl[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5019-74-9P, 2-Propanol, 1,1'-[[2-(5-nitro-2-furyl)-4-quinazolinyl]imino]di- 5019-76-1P, Quinazoline, 4-[[2-(diethylamino)ethyl]methylamino]-2-(5-nitro-2-furyl)-, hydrochloride 5019-78-3P, Quinazoline, 4-(1-methylhydrazino)-2-(5-nitro-2-furyl)- 5019-79-4P, Ethanol, 2-[1-[2-(5-nitro-2-furyl)-4-quinazolinyl]hydrazino]- 5055-17-4P, Ethanol, 2-[ethyl[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5055-18-5P, Ethanol, 2-[isopropyl[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5055-19-6P, Ethanol, 2-[butyl[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5055-20-9P, Ethanol, 2,2'-[[2-(5-nitro-2-furyl)-4-quinazolinyl]imino]di- 5055-21-0P, 2-Propanol, 1-[(2-hydroxyethyl)[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5055-23-2P, Quinazoline, 4-[3-(dimethylamino)propyl]amino]-2-(5-nitro-2-furyl)-, hydrochloride 5055-24-3P, Quinazoline, 4-[[2-(dimethylamino)ethyl]methylamino]-2-(5-nitro-2-furyl)-, hydrochloride 5055-25-4P, Quinazoline, 4-[[2-(diethylamino)ethyl]amino]-2-(5-nitro-2-furyl)-, hydrochloride 5055-28-7P, Quinazoline, 2-(5-nitro-2-furyl)-4-[[3-(1-pyrrolidinyl)propyl]amino]-, hydrochloride 5055-31-2P, Quinazoline, 4-[(3-methoxypropyl)amino]-2-(5-nitro-2-furyl)- 5055-33-4P, Quinazoline, 4-[bis(2-ethoxyethyl)amino]-2-(5-nitro-2-furyl)- 5085-66-5P, 1-Propanol, 3-[[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5094-03-1P, Ethanol, 2-[methyl[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5094-04-2P, Quinazoline, 2-(5-nitro-2-furyl)-4-[[4-(1-pyrrolidinyl)butyl]amino]-, hydrochloride 5118-19-4P, 1,2,3,4,5-Hexanepentol, 6-[methyl[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- 5489-93-0P, Quinazoline, 4-[(3-morpholinopropyl)amino]-2-(5-nitro-2-furyl)-, dihydrochloride 27465-08-3P, Quinazoline, 2-(5-nitro-2-furyl)-4-[[2-(1-pyrrolidinyl)ethyl]amino]-, hydrochloride 27465-09-4P, Quinazoline, 4-[[2-(dimethylamino)ethyl]amino]-2-(5-nitro-2-furyl)-, hydrochloride 27465-10-7P, Quinazoline, 4-[[3-(diethylamino)propyl]amino]-2-(5-nitro-2-furyl)-, hydrochloride

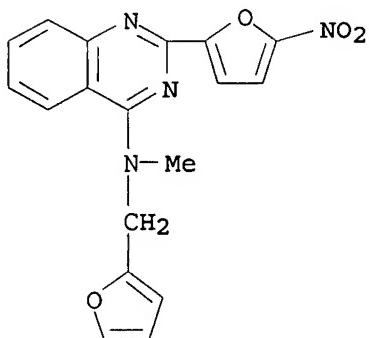
RL: PREP (Preparation)
 (preparation of)

RN 5019-67-0 ZCAPLUS
 CN 4-Quinazolinamine, 2-(5-nitro-2-furanyl)-N-[(tetrahydro-2-furanyl)methyl]-(9CI) (CA INDEX NAME)

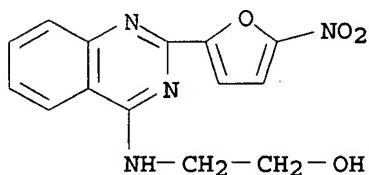


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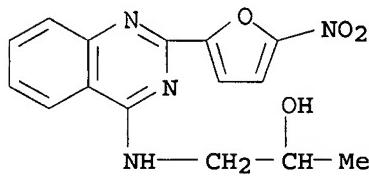
RN 5019-68-1 ZCPLUS
CN 4-Quinazolinamine, N-(2-furanylmethyl)-N-methyl-2-(5-nitro-2-furanyl)-
(9CI) (CA INDEX NAME)



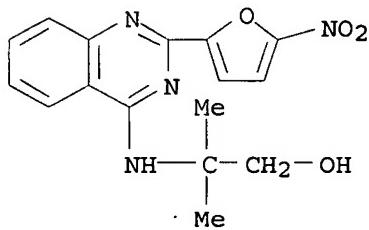
RN 5019-69-2 ZCPLUS
CN Ethanol, 2-[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



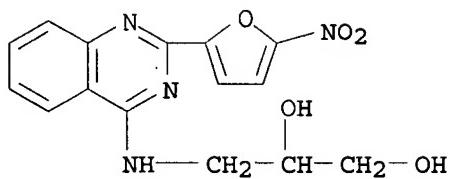
RN 5019-70-5 ZCPLUS
CN 2-Propanol, 1-[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



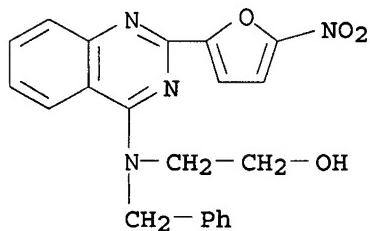
RN 5019-71-6 ZCPLUS
CN 1-Propanol, 2-methyl-2-[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]-
(9CI) (CA INDEX NAME)



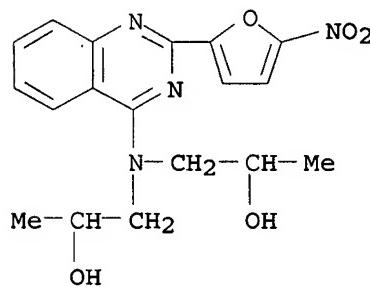
RN 5019-72-7 ZCPLUS
CN 1,2-Propanediol, 3-[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI)
(CA INDEX NAME)



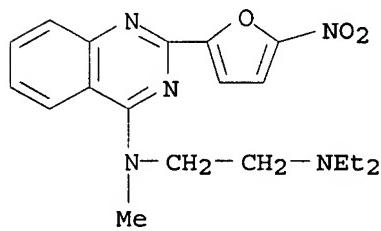
RN 5019-73-8 ZCPLUS
CN Ethanol, 2-[(2-(5-nitro-2-furanyl)-4-quinazolinyl) (phenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 5019-74-9 ZCPLUS
CN 2-Propanol, 1,1' - [(2-(5-nitro-2-furanyl)-4-quinazolinyl)imino]bis- (9CI) (CA INDEX NAME)



RN 5019-76-1 ZCPLUS
CN 1,2-Ethanediamine, N,N-diethyl-N-methyl-N-[2-(5-nitro-2-furanyl)-4-quinazolinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

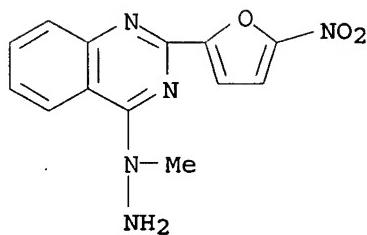


● HCl

RN 5019-78-3 ZCPLUS
CN Quinazoline, 4-(1-methylhydrazino)-2-(5-nitro-2-furanyl)- (9CI) (CA INDEX

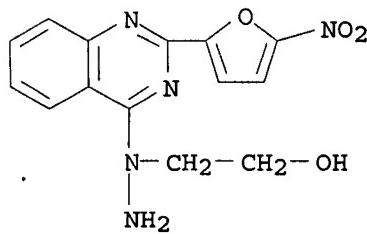
10 / 567,660

NAME)



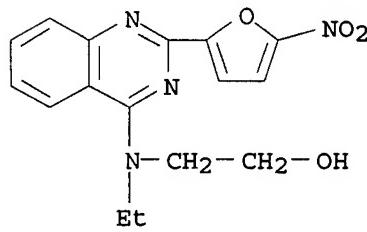
RN 5019-79-4 ZCPLUS

CN Ethanol, 2-[1-[2-(5-nitro-2-furanyl)-4-quinazolinyl]hydrazino]- (9CI) (CA INDEX NAME)



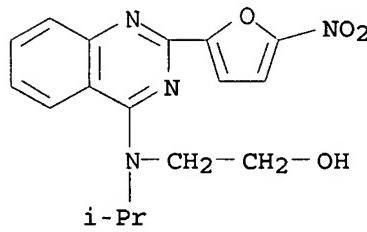
RN 5055-17-4 ZCPLUS

CN Ethanol, 2-[ethyl[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



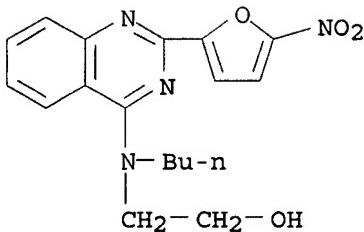
RN 5055-18-5 ZCPLUS

CN Ethanol, 2-[(1-methylethyl)[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

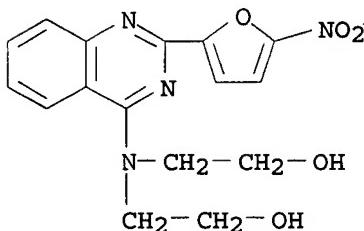


RN 5055-19-6 ZCPLUS

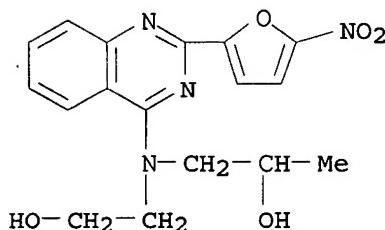
CN Ethanol, 2-[butyl[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



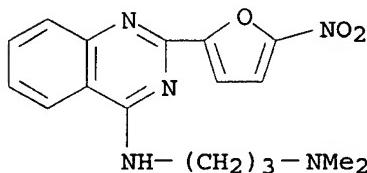
RN 5055-20-9 ZCPLUS
CN Ethanol, 2,2'-[[2-(5-nitro-2-furanyl)-4-quinazolinyl]imino]bis- (9CI) (CA INDEX NAME)



RN 5055-21-0 ZCPLUS
CN 2-Propanol, 1-[(2-hydroxyethyl) [2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

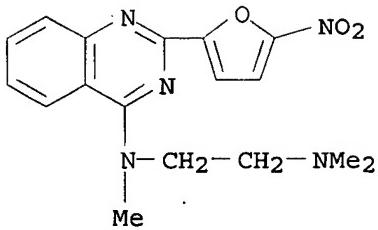


RN 5055-23-2 ZCPLUS
CN 1,3-Propanediamine, N,N-dimethyl-N'-(2-(5-nitro-2-furanyl)-4-quinazolinyl)- monohydrochloride (9CI) (CA INDEX NAME)



● HCl

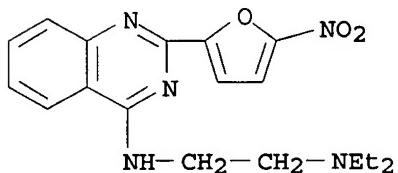
RN 5055-24-3 ZCPLUS
CN 1,2-Ethanediamine, N,N,N',N'-trimethyl-N'-(2-(5-nitro-2-furanyl)-4-quinazolinyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 5055-25-4 ZCPLUS

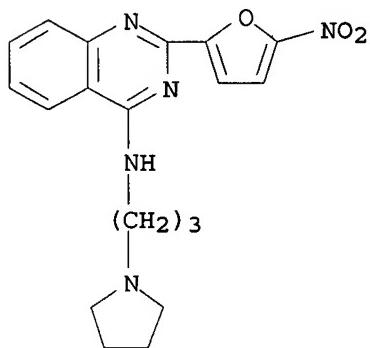
CN 1,2-Ethanediamine, N,N-diethyl-N'-(2-(5-nitro-2-furanyl)-4-quinazolinyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 5055-28-7 ZCPLUS

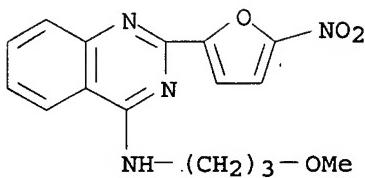
CN 4-Quinazolinamine, 2-(5-nitro-2-furanyl)-N-[3-(1-pyrrolidinyl)propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

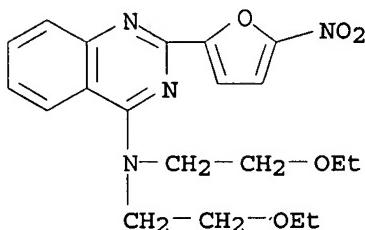
RN 5055-31-2 ZCPLUS

CN 4-Quinazolinamine, N-(3-methoxypropyl)-2-(5-(nitro-2-furanyl)- (9CI) (CA INDEX NAME)



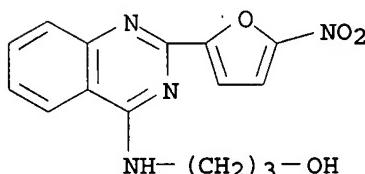
RN 5055-33-4 ZCPLUS

CN 4-Quinazolinamine, N,N-bis(2-ethoxyethyl)-2-(5-nitro-2-furanyl)- (9CI)
(CA INDEX NAME)



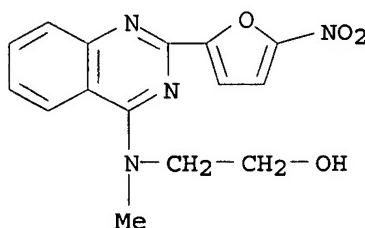
RN 5085-66-5 ZCPLUS

CN 1-Propanol, 3-[[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]- (9CI) (CA
INDEX NAME)



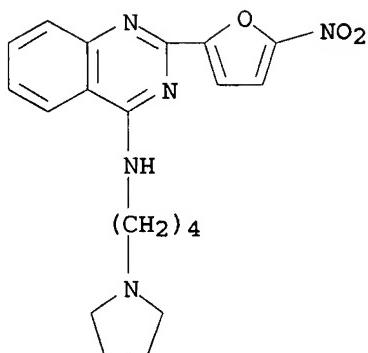
RN 5094-03-1 ZCPLUS

CN Ethanol, 2-[methyl[2-(5-nitro-2-furyl)-4-quinazolinyl]amino]- (9CI) (CA
INDEX NAME)



RN 5094-04-2 ZCPLUS

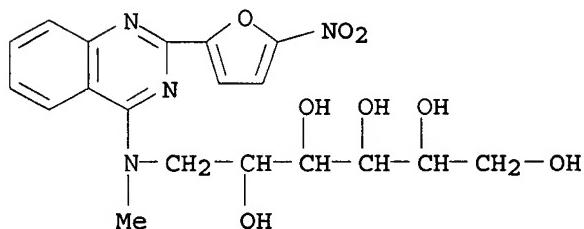
CN 4-Quinazolinamine, 2-(5-nitro-2-furyl)-N-[(4-(1-pyrrolidinyl)butyl)methyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

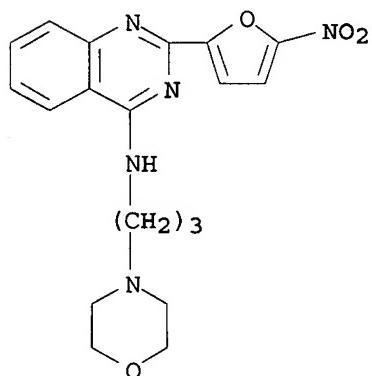
RN 5118-19-4 ZCPLUS

CN Hexitol, 1-deoxy-1-[methyl[2-(5-nitro-2-furanyl)-4-quinazolinyl]amino]-
(9CI) (CA INDEX NAME)



RN 5489-93-0 ZCPLUS

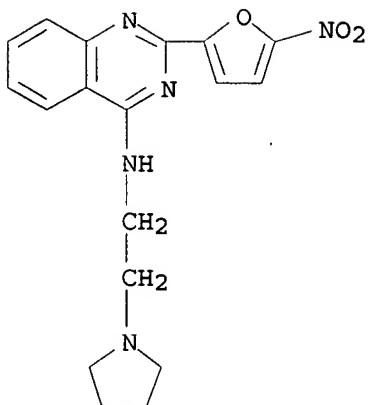
CN 4-Quinazolinamine, N-[3-(4-morpholinyl)propyl]-2-(5-nitro-2-furanyl)-,
dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 27465-08-3 ZCPLUS

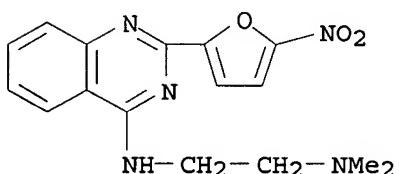
CN Quinazoline, 2-(5-nitro-2-furyl)-4-[[2-(1-pyrrolidinyl)ethyl]amino]-,
hydrochloride (7CI, 8CI) (CA INDEX NAME)



●x HCl

RN 27465-09-4 ZCPLUS

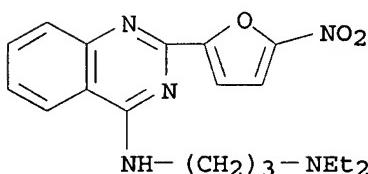
CN Quinazoline, 4-[(2-(dimethylamino)ethyl)amino]-2-(5-nitro-2-furyl)-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



●x HCl

RN 27465-10-7 ZCPLUS

CN Quinazoline, 4-[(3-diethylamino)propyl]amino]-2-(5-nitro-2-furyl)-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



●x HCl

ORIGINAL REFERENCE NO.: 45:3852g-i,3853a
 TITLE: Furylquinazolines. IV. Nucleophilic reactivity of the
 2-furyl-4-alkoxyquinazolines
 AUTHOR(S): Andrisano, R.; Modena, G.
 CORPORATE SOURCE: Univ. Bologna, Italy
 SOURCE: Bollettino Scientifico della Facolta di Chimica
 Industriale di Bologna (1950), 8, 7-9
 CODEN: BSFCAY; ISSN: 0366-3205

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

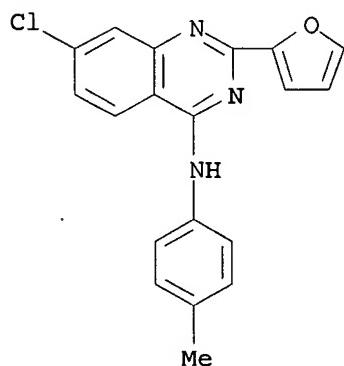
AB cf. preceding abstract 2-Furyl-4-chloroquinazoline (I) (C.A. 45, 1600f), refluxed for 0.5 hr. with 0.05 atom Na in 20-30 cc. of an aliphatic alc., poured into H₂O after cooling, and extracted with Et₂O, yields the corresponding 4-alkoxy derivative Thus, the following 2-furyl-4-alkoxyquinazolines (II) are prepared: MeO, prisms from ligroin, m. 65° (picrate, prisms from EtOH, m. 170°); EtO, needlelike prisms from ligroin, m. 83° (picrate, prisms from EtOH, m. 183.4°); PrO, characterized as the picrate, needlelike prisms from EtOH, m. 143.5°; iso-PrO, characterized as the picrate, prisms from EtOH, m. 164°. Similarly, by refluxing 0.02 mol. I, 0.05 atom Na, 8 cc. PhCH₂OH, and 20 cc. dioxane for 1 hr. was prepared 2-furyl-4-benzyloxyquinazoline (III), oil, characterized as the picrate, prisms from EtOH, m. 171°. Also, 2-furyl-4-phenoxyquinazoline (IV), prisms from ligroin, m. 135°. These compds. are hydrolyzed to 2-furyl-4-hydroxyquinazoline by refluxing with aqueous NaOH until they are completely dissolved; the rate of hydrolysis decreases in the order II > IV > III. Refluxing II, III, or IV with a Na alcoholate in the corresponding alc. or in dioxane yields the corresponding 4-alkoxy derivative In general, II are converted to their higher or lower homologs; IV easily yields II and III, but is not formed by this reaction. IV (3.3 g.) and 3 g. Et₂N(CH₂)₃CHMeNH₂ heated at 150° for 1.5 hrs., washed with 10% aqueous NaOH, and distilled in vacuo, yield 2-furyl-4-(5-diethylamino-2-pentylamino)quinazoline, characterized as the picrate, needles from EtOH, m. 179°.

IT 858236-39-2P, Quinazoline, 7-chloro-2-(2-furyl)-4-p-toluidino-
 858236-41-6P, Quinazoline, 7-chloro-2-(2-furyl)-4-phenetidino-
 860191-81-7P, Quinazoline, 4-(anisidino)-7-chloro-2-(2-furyl)-

RL: PREP (Preparation)
 (preparation of)

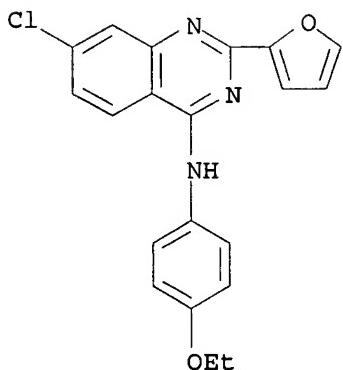
RN 858236-39-2 ZCAPLUS

CN Quinazoline, 7-chloro-2-(2-furyl)-4-p-toluidino- (5CI) (CA INDEX NAME)



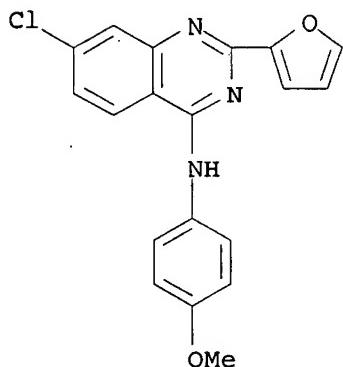
RN 858236-41-6 ZCAPLUS

CN Quinazoline, 7-chloro-2-(2-furyl)-4-phenetidino- (5CI) (CA INDEX NAME)



RN 860191-81-7 ZCPLUS

CN Quinazoline, 4-(anisidino)-7-chloro-2-(2-furyl)- (5CI) (CA INDEX NAME)



L4 ANSWER 38 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:21794 ZCPLUS

DOCUMENT NUMBER: 45:21794

ORIGINAL REFERENCE NO.: 45:3852c-g

TITLE: Furylquinazolines. III. 4-Substituted
2-furyl-4-chloroquinazolines

AUTHOR(S): Andrisano, R.; Modena, G.

CORPORATE SOURCE: Univ., Bologna, Italy

SOURCE: Gazzetta Chimica Italiana (1950), 80, 321-4

CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 45:21794

AB cf. C.A. 45, 1601d; following abstract In view of the high anti-malarial power of 4-(4-diethylamino-1-methylbutylamino)-7-chloroquinazoline (cf. Price, et al., C.A. 40, 5747.4), its 2-(2-furyl) derivative (I) was prepared 4,2-Cl(H₂N)C₆H₃CO₂H (10 g.) and 12 g. Et 2-furancarboximidate [cf. Ber. 25, 1416(1892)], heated 2 hrs. at 200°, the product taken up in MeOH, filtered, and the residue purified by AcOH, yield 2-(2-furyl)-4-hydroxy-7-chloroquinazoline (II), m. 276°. II (10 g.) in 80 cc. POCl₃ and 14 g. PCl₅, refluxed 90 min., distilled in vacuo, the residue taken up in ice water, neutralized with NH₄OH, filtered, and the residue extracted with C₆H₆, yields 9.5 g. (88%) of 2-(2-furyl)-4,7-dichloroquinazoline (III), m. 137°. III (5.3 g.) and 6.4 g. H₂NCHMeCH₂CH₂NET₂ in 80 cc. C₆H₆, neutralized by Na₂CO₃, refluxed 3 hrs., and the product steam-distilled, yield almost 100 % I, m. 112°. With alc. picric acid, it forms a picrate, C₃₃H₃₃O₁₅N₁₀Cl, m. 199°.

Since the Cl in the 4-position in III, like that in the chloroquinazolines already described (cf. C.A. 45, 1600f) is reactive with nucleophilic agents, 6 compds. were prepared by replacement of the Cl. III (0.01 mol.) and NaOMe (from 0.03 atom Na in 40 cc. MeOH), refluxed 30 min., diluted with water, and the precipitate purified by ligroin, yields 2-(2-furyl)-4-methoxy-7-chloroquinazoline, m. 130°. III (0.01 mol.) in 20 cc. dioxane and NaOPh (from 0.03 atom Na in 12 g. PhOH), refluxed 30 min., poured into water, NaOH added, and the precipitate purified by aqueous EtOH, yield 100% of the

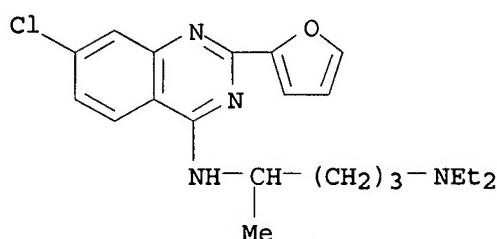
4-phenoxy analog, m. 140°. Four arylamino derivs. were prepared in high yields by refluxing 0.01 mol. III and 0.02 mol. of the resp. arylamine 1 hr. in C6H6, making alkaline with Na2CO3, and steam-distilling 2-(2-Furyl)-4-phenylamino-7-chloroquinazoline, m. 170° (from EtOH); 4-tolylamino analog, m. 201° (from ligroin); 4-methoxyphenylamino analog, m. 189° (from EtOH); 4-ethoxyphenylamino analog, m. 180° (from EtOH).

IT 858235-29-7P, Quinazoline, 7-chloro-4-(4-diethylamino-1-methylbutylamino)-2-(2-furyl)- 860191-83-9P, Quinazoline, 4-anilino-7-chloro-2-(2-furyl)-

RL: PREP (Preparation)
(preparation of)

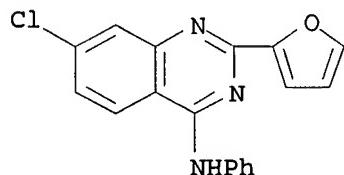
RN 858235-29-7 ZCPLUS

CN Quinazoline, 7-chloro-4-(4-diethylamino-1-methylbutylamino)-2-(2-furyl)-(5CI) (CA INDEX NAME)



RN 860191-83-9 ZCPLUS

CN Quinazoline, 4-anilino-7-chloro-2-(2-furyl)-(5CI) (CA INDEX NAME)



L4 ANSWER 39 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:8789 ZCPLUS

DOCUMENT NUMBER: 45:8789

ORIGINAL REFERENCE NO.: 45:1601c-g

TITLE: Furylquinazolines. II. 4-Substituted
2-furyl-6-methylquinazolines

AUTHOR(S): Andrisano, R.; Modena, G.

CORPORATE SOURCE: Univ., Bologna, Italy

SOURCE: Bollettino Scientifico della Facolta di Chimica
Industriale di Bologna (1950), 8, 1-3

CODEN: BSFCAY; ISSN: 0366-3205

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. preceding abstract 5,2-Me(H2N) C6H3CO2Me (22 g.) and 24 g. Et

2-furanacetimidate (cf. Pinner, Ber. 25, 1416(1892)), heated at 200° for 1.5 hrs., taken up in MeOH after cooling, filtered, washed, and dried, yield 18.5 g. (61%) 2-furyl-4-hydroxy-6-methylquinazoline (I), silky needles from EtOH, m. 257°. I (16.8 g.) is refluxed with 100 cc. POCl₃ and 24 g. PCl₅ for 1.5 hrs., the excess POCl₃PCl₅ removed under reduced pressure, the residue taken up with H₂O and ice, neutralized with NH₄OH, filtered, washed, and dried to yield after recrystn. from C₆H₆ 14 g. (77%) 4-Cl analog (II), prisms from ligroin, m. 144°. Refluxing 5 g. II and 6.5 g. Et₂N(CH₂)₃CHMeNH₂ in 75 cc. C₆H₆, and removing the C₆H₆ and excess base with steam gives in almost quant. yield the 4-(5-diethylamino-2-pentylamino) analog, needles, b.p. 280°, m. 144° (from ligroin); picrate, needles from EtOH, m. 180°. II (0.01 mol.), refluxed with 0.03 atom Na in 40 cc. MeOH for 0.5 hr. and poured into H₂O, yields almost quantitatively the 4-MeO analog, colorless prisms from ligroin, m. 116°. Similarly, 0.01 mol. II, 0.03 atom Na, and 12 g. PhOH in 20 cc. dioxane give the 4-PhO analog, colorless prisms from ligroin, m. 141°. The following 2-furyl-4-arylamino-6-methylquinazolines are obtained in almost quant. yield by refluxing 0.01 mol. II with 0.02 mol. of the corresponding arylamine in 40 ml. C₆H₆, making alkaline with Na₂CO₃, and removing the solvent and excess amine with steam: PhNH, needles from aqueous EtOH, m. 180°; MeC₆H₄NH, needles from EtOH, m. 140°; p-MeOC₆H₄NH, needles from ligroin, m. 156°; p-EtOC₆H₄NH, silky needles from MeOH, m. 126°.

IT 857760-27-1P, Quinazoline, 4-(4-diethylamino-1-methylbutylamino)-2-

(2-furyl)-6-methyl- 860191-75-9P, Quinazoline,

4-(anisidino)-2-(2-furyl)-6-methyl- 860720-50-9P, Quinazoline,

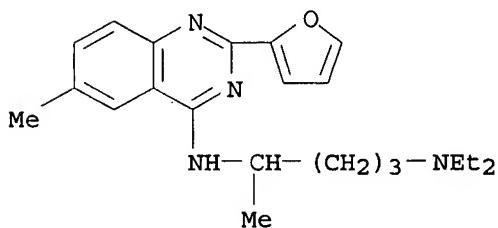
4-anilino-2-(2-furyl)-6-methyl-

RL: PREP (Preparation)

(preparation of)

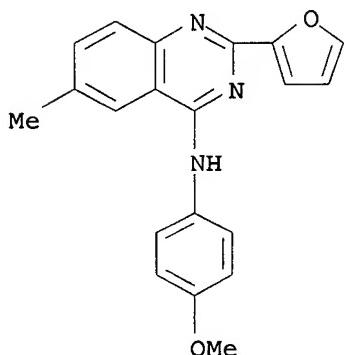
RN 857760-27-1 ZCAPLUS

CN Quinazoline, 4-(4-diethylamino-1-methylbutylamino)-2-(2-furyl)-6-methyl- (5CI) (CA INDEX NAME)

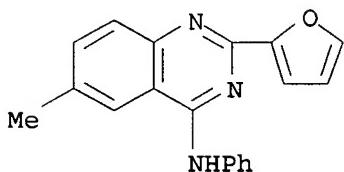


RN 860191-75-9 ZCAPLUS

CN Quinazoline, 4-(anisidino)-2-(2-furyl)-6-methyl- (5CI) (CA INDEX NAME)



RN 860720-50-9 ZCPLUS
 CN Quinazoline, 4-anilino-2-(2-furyl)-6-methyl- (5CI) (CA INDEX NAME)



L4 ANSWER 40 OF 40 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:8788 ZCPLUS

DOCUMENT NUMBER: 45:8788

ORIGINAL REFERENCE NO.: 45:1600f-i,1601a-c

TITLE: Furylquinazolines. I. 4-Substituted
2-furylquinazolines

AUTHOR(S): Andrisano, Renato; Modena, G.

CORPORATE SOURCE: Univ. Bologna, Italy

SOURCE: Gazzetta Chimica Italiana (1950), 80, 228-33
CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. following abstract In view of the plasmocidal action of quinazoline derivs. containing a pentylamine side chain (cf. Endicott, et al., C.A. 40, 5748.3; Price, et al., C.A. 40, 5747.4), some 2-furylquinazoline derivs. were prepared to study their anti-malarial activity and the comparative influence on their pharmacol. properties of the Ph and furan ring in the quinazoline nucleus. o-H₂NC₆H₄CO₂Me (20 g.) and 20 g.

OC₄H₃C(:NH)OEt [cf. Ber. 25, 1416(1892)], heated 3 hrs. at 210-20°, taken up in MeOH, filtered, and the residue purified by EtOH, yields 74% of 2-furyl-4-hydroxyquinazoline (I), m. 220°. Also, 10.3 g.

o-H₂NC₆H₄CO₂H and 9.5 g. OC₄H₃C(:S)NH₂ [Hantzsch, Ber. 25, 1314(1892)], heated at 150° until no more H₂S is evolved, and the product treated as before, yield approx. 74% I. I (10 g.) in 80 cc. POCl₃ and 14 g. PCl₅, heated 100 min. (no temperature given), distilled in vacuo, the residue neutralized with NH₄OH, mixed with ice water, and the crystallized product dried and extracted with C₆H₆, yield 9 g. (80%) of 2-furyl-4-chloroquinazoline (II). Hydrolysis by 5% alc. KOH yields I. II (4.1 g.) and 5 g. H₂NCHMe(CH₂)₃NET₂ in 60 cc. C₆H₆, refluxed 3 hrs., made alkaline with Na₂CO₃, and steam-distilled, leave a pasty residue which could

not

be crystallized even after distillation in vacuo (b16 286°). However, with alc. picric acid it formed, after purification by EtOH, a dipicrate, C₃₃H₃₄O₁₅N₁₀, m. 179°, and with H₃PO₄ a monohydrated diphosphate, C₂₁H₃₆O₁₀N₄P₂, m. 210°. The wts. of these corresponded to an almost 100% yield of 2-furyl-4-(4-diethylamino-1-methylbutylamino)quinazoline (III). III is also formed by the same procedure, but in the presence of PhOH without solvent. II (0.01 mol.) and alc. NaOMe (from 0.03 atom Na in 40 cc. MeOH), refluxed 1 hr., diluted with water, extracted with Et₂O, the extract evaporated, and the oil residue

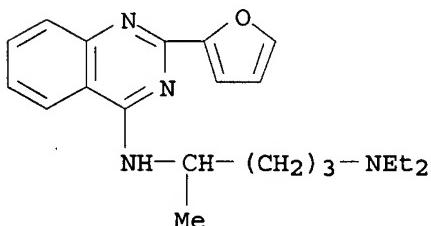
distilled

in vacuo (b16 212°), give, after purification by ligroin, a good yield of 2-furyl-4-methoxyquinazoline, m. 65°. II (0.01 mol.) and NaOPh (from 0.03 atom Na, 12 g. PhOH, and 20 cc. dioxane), refluxed 1 hr., poured into water, and NaOH added, give, after purification by ligroin, almost 100% of 2-furyl-4-phenoxyquinazoline (IV), m. 135°. Alc. II, treated while refluxing with anhydrous NH₃ for 1 hr., diluted with water, and the precipitate purified by EtOH, yields almost 100% 2-furyl-4-aminoquinazoline, m. 225°. II (0.01 mol.) in C₆H₆ and 0.02 mol. of

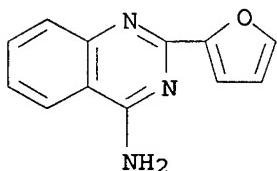
arylamine in 40 cc. C₆H₆, refluxed 1 hr., made alkaline with Na₂CO₃, steam-distilled, and the residues purified by EtOH, yielded almost 100% of the following 2-furyl-4-(arylamino)quinazolines: NHPh, m. 115°; NHC₆H₄Me, m. 133°; NHC₆H₄OMe, m. 110°; NHC₆H₄OEt, m.

105°. The extreme reactivity of the Cl in II is similar to the behavior of Cl in 2,4,1-(O₂N)C₁₀H₅Cl (cf. Mangini and Frenguelli, C.A. 32, 1258.3) and the Cl in 4-chloroquinazoline (cf. Tomisek and Christiensen, C.A. 32, 1259.1). This is in harmony with the theory of Bonino and the expts. of Mangini and Frenguelli (Atti accad. sci. Bologna [10] 1, 201(1944); C.A. 33, 5398.6), and of the pharmacol. expts. of Erlenmeyer (C.A. 41, 1671g) concerning the analogy between the heterocyclic N atom and the aromatic CNO₂ group, which, by strongly polarizing the electronic cloud in relation to the nuclear CCl group, increase the tendency toward replacement of the Cl.

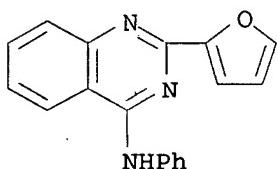
- IT 857760-25-9, Quinazoline, 4-(4-diethylamino-1-methylbutylamino)-2-(2-furyl)-
(and derivs.)
RN 857760-25-9 ZCPLUS
CN Quinazoline, 4-(4-diethylamino-1-methylbutylamino)-2-(2-furyl)- (5CI) (CA INDEX NAME)



- IT 40172-85-8P, Quinazoline, 4-amino-2-(2-furyl)-
157863-04-2P, Quinazoline, 4-anilino-2-(2-furyl)-
860191-77-1P, Quinazoline, 4-(anisidino)-2-(2-furyl)-
RL: PREP (Preparation)
(preparation of)
RN 40172-85-8 ZCPLUS
CN 4-Quinazolinamine, 2-(2-furanyl)- (9CI) (CA INDEX NAME)



- RN 157863-04-2 ZCPLUS
CN 4-Quinazolinamine, 2-(2-furanyl)-N-phenyl- (9CI) (CA INDEX NAME)



- RN 860191-77-1 ZCPLUS
CN Quinazoline, 4-(anisidino)-2-(2-furyl)- (5CI) (CA INDEX NAME)